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| | | |
|---|---|---|
| NEWS 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS 2 | | "Ask CAS" for self-help around the clock |
| NEWS 3 | AUG 09 | INSPEC enhanced with 1898-1968 archive |
| NEWS 4 | AUG 28 | ADISCTI Reloaded and Enhanced |
| NEWS 5 | AUG 30 | CA(SM)/CAplus(SM) Austrian patent law changes |
| NEWS 6 | SEP 21 | CA/CAplus fields enhanced with simultaneous left and right truncation |
| NEWS 7 | SEP 25 | CA(SM)/CAplus(SM) display of CA Lexicon enhanced |
| NEWS 8 | SEP 25 | CAS REGISTRY(SM) no longer includes Concord 3D coordinates |
| NEWS 9 | SEP 25 | CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine |
| NEWS 10 | SEP 28 | CEABA-VTB classification code fields reloaded with new classification scheme |
| NEWS 11 | OCT 19 | LOGOFF HOLD duration extended to 120 minutes |
| NEWS 12 | OCT 19 | E-mail format enhanced |
| NEWS 13 | OCT 23 | Option to turn off MARPAT highlighting enhancements available |
| NEWS 14 | OCT 23 | CAS Registry Number crossover limit increased to 300,000 in multiple databases |
| NEWS 15 | OCT 23 | The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded |
| NEWS 16 | OCT 30 | CHEMLIST enhanced with new search and display field |
| NEWS 17 | NOV 03 | JAPIO enhanced with IPC 8 features and functionality |
| NEWS 18 | NOV 10 | CA/CAplus F-Term thesaurus enhanced |
| NEWS 19 | NOV 10 | STN Express with Discover! free maintenance release Version 8.01c now available |
| NEWS 20 | NOV 20 | CAS Registry Number crossover limit increased to 300,000 in additional databases |
| NEWS 21 | NOV 20 | CA/CAplus to MARPAT accession number crossover limit increased to 50,000 |
| NEWS 22 | DEC 01 | CAS REGISTRY updated with new ambiguity codes |
| NEWS 23 | DEC 11 | CAS REGISTRY chemical nomenclature enhanced |
| NEWS 24 | DEC 14 | WPIDS/WPINDEX/WPIX manual codes updated |
| NEWS 25 | DEC 14 | GBFULL and FRFULL enhanced with IPC 8 features and functionality |
| NEWS 26 | DEC 18 | CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role |
| NEWS 27 | DEC 18 | CA/CAplus patent kind codes updated |
| NEWS 28 | DEC 18 | MARPAT to CA/CAplus accession number crossover limit increased to 50,000 |
| NEWS 29 | DEC 18 | MEDLINE updated in preparation for 2007 reload |
| NEWS 30 | DEC 27 | CA/CAplus enhanced with more pre-1907 records |

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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 NEWS HOURS     STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN     Welcome Banner and News Items
 NEWS IPC8      For general information regarding STN implementation of IPC 8
 NEWS X25       X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
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FILE 'HOME' ENTERED AT 07:49:52 ON 08 JAN 2007

=> file reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 07:50:03 ON 08 JAN 2007
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STRUCTURE FILE UPDATES:  7 JAN 2007  HIGHEST RN 916885-50-2
DICTIONARY FILE UPDATES:  7 JAN 2007  HIGHEST RN 916885-50-2

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 4.str
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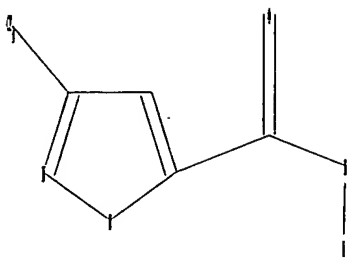

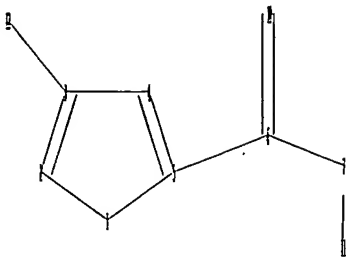

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6 7 10 11 12
ring nodes :
1 2 3 4 5
chain bonds :
3-12 5-6 6-7 6-10 7-11
ring bonds :
1-5 1-2 2-3 3-4 4-5
exact/norm bonds :
1-5 1-2 2-3 3-4 4-5 6-7 6-10
exact bonds :
3-12 5-6 7-11

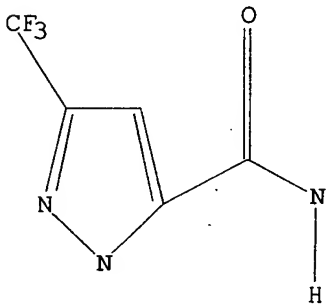
G1:Cb,Cy,Hy

G2:S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 10:CLASS 11:CLASS
12:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR




G1 Cb,Cy,Hy
G2 S,N

Structure attributes must be viewed using STN Express query preparation.

10519356a.trn

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SAMPLE SEARCH INITIATED 07:50:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      165 TO ITERATE

100.0% PROCESSED      165 ITERATIONS                          50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          2530 TO     4070
PROJECTED ANSWERS:             1761 TO     3079

L2            50 SEA SSS SAM L1

=> d scan
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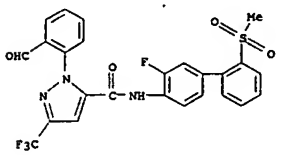
L2 50 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-(2-formylphenyl)-3-(trifluoromethyl)- (9CI)
MF C25 H17 F4 N3 O4 S




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus
COST IN U.S. DOLLARS

| | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.45 | 0.66 |

FILE 'CAPLUS' ENTERED AT 07:50:41 ON 08 JAN 2007
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FILE COVERS 1907 - 8 Jan 2007 VOL 146 ISS 3
FILE LAST UPDATED: 7 Jan 2007 (20070107/ED)

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http://www.cas.org/infopolicy.html

=> l2
L3 28 L2

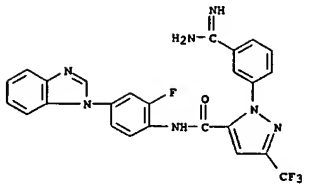
=> d ibib abs hitstr 20-28

L3 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:791919 CAPLUS
DOCUMENT NUMBER: 141:342889
TITLE: SAR and factor IXa crystal structure of a dual inhibitor of factors IXa and Xa
AUTHOR(S): Smallheer, Joanne M.; Alexander, Richard S.; Wang, Jianmin; Wang, Shuaige; Nakajima, Suanne; Rossi, Karen A.; Smallwood, Angela; Barbera, Frank; Burdick, Debra; Luettgen, Joseph M.; Knabb, Robert M.; Wexler, Ruth R.; Jadhav, Prabhakar K.
CORPORATE SOURCE: Bristol-Myers Squibb Company, Princeton, NJ, 08543-5400, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(21), 5263-5267
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:342889
AB Modifications to the P4 moiety and pyrazole C3 substituent of factor Xa inhibitor SN-429 provided several new compds., which are 5-10 nM inhibitors of factor IXa. An x-ray crystal structure of one example complexed to factor IXa shows that these compds. adopt a similar binding mode to that previously observed with pyrazole inhibitors in the factor Xa active site both with regard to how the inhibitor binds and the position of Tyr99.
IT 848393-63-5P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(pyrazole compds. preparation, crystal structure, and dual inhibition of factors IXa and Xa)
RN 848393-63-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-46-1
CMF C25 H17 F4 N7 O

L3 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

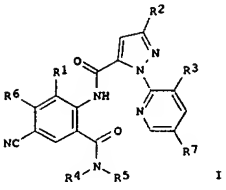
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:648522 CAPLUS
DOCUMENT NUMBER: 141:190786
TITLE: Preparation of cyano anthranilamide insecticides
INVENTOR(S): Hughes, Kenneth Andrew; Lahm, George Philip; Selby, Thomas Paul; Stevenson, Thomas Martin
PATENT ASSIGNEE(S): E.I. Du Pont De Nemours and Company, USA
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004067528 | A1 | 20040812 | WO 2004-US3568 | 20040121 |
| WO 2004067528 | B1 | 20041007 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI | | | | |
| AU 2004207848 | A1 | 20040812 | AU 2004-207848 | 20040121 |
| CA 2512242 | A1 | 20040812 | CA 2004-2512242 | 20040121 |
| EP 1599463 | A1 | 20051130 | EP 2004-704148 | 20040121 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| MD 2005000219 | A | 20051130 | MD 2005-219 | 20040121 |
| BR 2004006709 | A | 20051220 | BR 2004-6709 | 20040121 |
| JP 3764895 | B1 | 20060412 | JP 2005-518229 | 20040121 |
| JP 2006515602 | T | 20060601 | | |
| CN 1829707 | A | 20060906 | CN 2004-80002991 | 20040121 |
| EG 23536 | A | 20060419 | EG 2004-49 | 20040127 |
| JP 2006028159 | A | 20060202 | JP 2005-148184 | 20050520 |
| JP 3770500 | B2 | 20060426 | | |
| JP 2006290862 | A | 20061026 | JP 2005-148201 | 20050520 |
| US 2006111403 | A1 | 20060525 | US 2005-540966 | 20050629 |
| PRIORITY APPLN. INFO.: | | | US 2003-443256P P | 20030128 |
| | | | JP 2005-518229 A3 | 20040121 |
| | | | WO 2004-US3568 W | 20040121 |

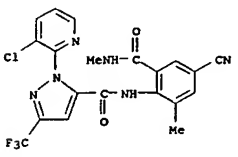
OTHER SOURCE(S): MARPAT 141:190786
GI

L3 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



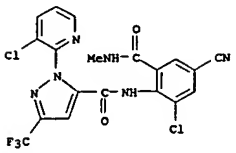
I

AB The title compds. [I; R1 = Me, Cl, Br, F; R2 = F, Cl, Br, haloalkyl or haloalkoxy; R3 = F, Cl, Br; R4 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, each optionally substituted with one substituent selected from the group consisting of halo, CN, SMe S(O)Me, S(O)2Me and OMe; R5 = H, Me; R6 = H, F, Cl; R7 = H, F, Cl], useful for controlling an invertebrate pest, were prepared E.g., a multi-step synthesis of compound I [R1 = Me; R2 = CF3; R3 = Cl; R4, R5 = H], was given. The compds. I were tested in various biol. tests (data given). This invention also pertains to a composition for controlling an invertebrate pest comprising a biol. effective amount of a compound I, an N-oxide thereof or a suitable salt of the compound I and at least one addnl. component selected from the group consisting of a surfactant, a solid diluent and a liquid diluent.
IT 736994-60-8P 736994-79-9P 736994-94-8P 736995-07-6P 736995-09-8P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyano anthranilamide insecticides)
RN 736994-60-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-[4-cyano-2-methyl-6-[(methylamino)carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

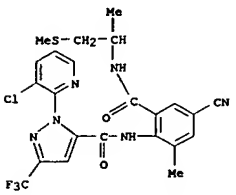


RN 736994-79-9 CAPLUS

L3 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, N-[2-chloro-4-cyano-6-[(methylamino)carbonyl]phenyl]-1-(3-chloro-2-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

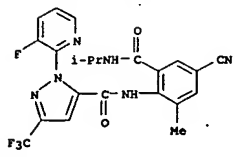


RN 736994-94-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-[4-cyano-2-methyl-6-[[[1-methyl-2-(methylthio)ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

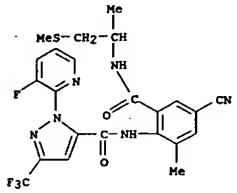


RN 736995-07-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-cyano-2-methyl-6-[[(1-methylethyl)amino]carbonyl]phenyl]-1-(3-fluoro-2-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

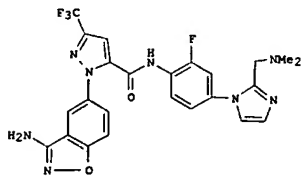
L3 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 736995-09-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-cyano-2-methyl-6-[[[1-methyl-2-(methylthio)ethyl]amino]carbonyl]phenyl]-1-(3-fluoro-2-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



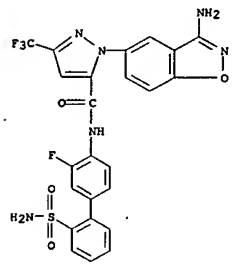
L3 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:566937 CAPLUS
DOCUMENT NUMBER: 142:219198
TITLE: Discovery of 1-(3'-Aminobenzisoxazol-5'-yl)-3-trifluoromethyl-N-[2-fluoro-4-[(2'-dimethylaminomethyl)imidazol-1-yl]phenyl]-1H-pyrazole-5-carboxyamide Hydrochloride (Razaxaban), a Highly Potent, Selective, and Orally Bioavailable Factor Xa Inhibitor
AUTHOR(S): Quan, Mimi L.; Lam, Patrick Y. S.; Han, Qi; Pinto, Donald J. P.; He, Ming Y.; Li, Renhua; Ellis, Christopher D.; Clark, Charles G.; Teleha, Christopher A.; Sun, Jung-Hui; Alexander, Richard S.; Bai, Steve; Luettgen, Joseph M.; Knabb, Robert M.; Wong, Pancras C.; Wexler, Ruth R.
CORPORATE SOURCE: Discovery Chemistry Pharmaceutical Research Institute, Bristol-Myers Squibb Co., Princeton, NJ, 08543-5400, USA
SOURCE: Journal of Medicinal Chemistry (2005), 48(6), 1729-1744
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:219198
GI



I

AB Modification of a series of pyrazole factor Xa inhibitors to incorporate an aminobenzisoxazole as the P1 ligand resulted in compds. with improved selectivity for factor Xa relative to trypsin and plasma kallikrein. Further optimization of the P4 moiety led to compds. with enhanced permeability and reduced protein binding. The SAR and pharmacokinetic profile of this series of compds. is described. These efforts culminated in 1-(3'-aminobenzisoxazol-5'-yl)-3-trifluoromethyl-N-[2-fluoro-4-[(2'-dimethylaminomethyl)imidazol-1-yl]phenyl]-1H-pyrazole-5-carboxamide (I), a potent, selective, and orally bioavailable inhibitor of factor Xa. On the basis of its excellent in vitro potency and selectivity profile, high free fraction in human plasma, good oral bioavailability, and in vivo efficacy

L3 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
in antithrombotic models, the HCl salt of this compd. was selected for clin. development as razaxaban (DPC 906, BMS-561389).
IT 754193-63-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of razaxaban and related compds. as potent, selective, and orally bioavailable factor Xa inhibitors)
RN 754193-63-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



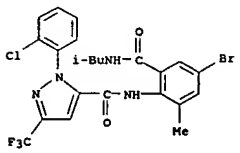
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:270097 CAPLUS
DOCUMENT NUMBER: 140:282468
TITLE: Cloning and characterization of insect ryanodine receptors and their use for screening for insecticidal compounds
INVENTOR(S): Caspar, Timothy; Cordova, Daniel; Gutteridge, Steven; Rauh, James J.; Smith, Rejane M.; Wu, Lihong; Tao, Yong
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours and Company, USA
SOURCE: PCT Int. Appl., 731 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004027042 | A2 | 20040401 | WO 2003-US29834 | 20030923 |
| WO 2004027042 | A3 | 20041118 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2003275128 | A1 | 20040408 | AU 2003-275128 | 20030923 |
| US 2004171114 | A1 | 20040902 | US 2003-668767 | 20030923 |
| EP 1546183 | A2 | 20050629 | EP 2003-759396 | 20030923 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| JP 2006516884 | T | 20060713 | JP 2004-538401 | 20030923 |
| PRIORITY APPLN. INFO.: | | | US 2002-412795P | P 20020923 |
| | | | US 2002-427324P | P 20021118 |
| | | | WO 2003-US29834 | W 20030923 |

AB The genes encoding ryanodine receptor homologs are provided from multiple insect families including lepidopteran tobacco budworm (Heliothis virescens), homopteran green peach aphid (Myzus persicae), corn plant hopper (Peregrinus maidis), cotton melon aphid (Aphis gossypii), and fruitfly (Drosophila melanogaster). The full-length genes were isolated, cloned, and amplified in bacterial cells. Expression in insect cells shows that the recombinant protein folds into a functional calcium release channel. The genes and their corresponding polypeptides have a number of uses including, but not limited to, the isolation of other pest ryanodine receptors, the development of screens to identify insecticidally active compds., use of fragments of genes as pesticides, fragments of protein for

L3 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
antibody prodn., fragments of protein for detn. of the structure of insecticide binding sites, and identification of insecticides that disrupt the calcium balance in cells through other messengers that interact with the receptor calcium release mechanism. Methods are outlined for overcoming toxic effects of expressing recombinant proteins in host cells.
IT 675826-03-6
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(cloning and characterization of insect ryanodine receptors and their use for screening for insecticidal compds.)
RN 675826-03-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-bromo-2-methyl-6-[[(2-methylpropyl)amino]carbonyl]phenyl]-1-(2-chlorophenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

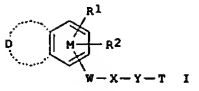



L3 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:20490 CAPLUS
DOCUMENT NUMBER: 140:77148
TITLE: Preparation of N-[4-(thiooxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis
INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsaklakidis, Christos; Gleitz, Johannes; Barnes, Christopher
PATENT ASSIGNEE(S): Merck Patent Gmbh, Germany
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004002477 | A1 | 20040108 | WO 2003-EP5898 | 20030605 |
| WO 2004002477 | A8 | 20040415 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| DE 10229070 | A1 | 20040115 | DE 2002-10229070 | 20020628 |
| CA 2491271 | A1 | 20040108 | CA 2003-2491271 | 20030605 |
| AU 2003238475 | A1 | 20040119 | AU 2003-238475 | 20030605 |
| EP 1517685 | A1 | 20050330 | EP 2003-732540 | 20030605 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| JP 2005535630 | T | 20051124 | JP 2004-516575 | 20030605 |
| EP 1679073 | A1 | 20060712 | EP 2006-157 | 20030605 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, SK | | | | |
| US 2005203127 | A1 | 20050915 | US 2004-519356 | 20041228 |
| PRIORITY APPLN. INFO.: | | | DE 2002-10229070 | A 20020628 |
| | | | EP 2003-732540 | A3 20030605 |
| | | | WO 2003-EP5898 | W 20030605 |

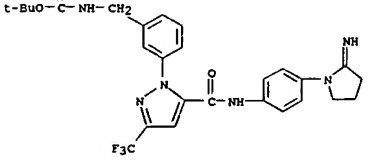
OTHER SOURCE(S): MARPAT 140:77148
GI

L3 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)




I

AB Title compds. [I; D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene; M = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(:S)N(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bi)cyclic aromatic (hetero)cyclyl; X = CONR3, CONR3C(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y = alkylene, cycloalkylene, heterodiyl, aryldiyl; T = (substituted) (bi)cyclic aromatic heterocyclyl], were prepared Thus, 333 mg (3-[5-(4-[2-iminopyrrolidin-1-yl]phenylcarbamoyl)-3-trifluoromethylpyrazol-1-yl]benzyl)carbamic acid tert-Bu ester (preparation given) in EtOH was treated with HCl in ether to give 289 mg N-[4-(2-iminopyrrolidin-1-yl)phenyl]-1-(3-aminomethylphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the receptor Xa with IC50 = 9,6·10-9 M and to the receptor VIIa with IC50 = 2,3·10-8 M.
IT 640288-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)
RN 640288-00-2 CAPLUS
CN Carbamic acid, [[3-[5-[[[4-(2-imino-1-pyrrolidinyl)phenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)




REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS

L3 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

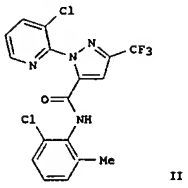
L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:1006958 CAPLUS
DOCUMENT NUMBER: 140:42172
TITLE: Preparation of pyrazolecarboxamide insecticides
INVENTOR(S): Stevenson, Thomas Martin; Lahm, George Philip; Pasteris, Robert James
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003106427 | A2 | 20031224 | WO 2003-US18609 | 20030610 |
| WO 2003106427 | A3 | 20040624 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2003245464 | A1 | 20031231 | AU 2003-245464 | 20030610 |
| EP 1511733 | A2 | 20050309 | EP 2003-739103 | 20030610 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| BR 2003011707 | A | 20050315 | BR 2003-11707 | 20030610 |
| CN 1659160 | A | 20050824 | CN 2003-812731 | 20030610 |
| JP 2005532367 | T | 20051027 | JP 2004-513260 | 20030610 |
| US 2006167060 | A1 | 20060727 | US 2004-514183 | 20041110 |

PRIORITY APPLN. INFO.: US 2002-388244P P 20020613
WO 2003-US18609 W 20030610

OTHER SOURCE(S): MARPAT 140:42172
GI

L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

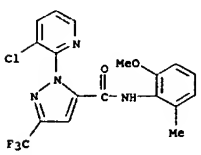


II

AB The title compds. BNR1C(:A)J [I; A = O, S; B = (un)substituted Ph, pyridinyl; J = pyrazole or pyrrole heterocyclic ring; R1 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl], useful for controlling at least one invertebrate pest (comprising contacting the invertebrate pest or its environment with a biol. effective amount of at least one compound I), were prepared E.g., a 3-step synthesis of II (starting from 2,3-dichloropyridine and 3-trifluoromethylpyrazole), was given. The compds. I were tested in 5 different tests against diamond moth, fall armyworm, tobacco budworm and beet armyworm, and biol. data were given. This invention also pertains to a composition comprising at least one compound I and at least one addnl. component selected from the group consisting of a surfactant, a solid diluent and a liquid diluent.

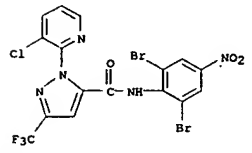
IT 636609-04-6P 636609-11-5P 636609-17-1P
636609-27-3P 636609-35-3P 636609-50-2P
636609-59-1P 636609-70-6P 636609-89-7P
636609-95-5P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolecarboxamide insecticides)

RN 636609-04-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2-methoxy-6-methylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

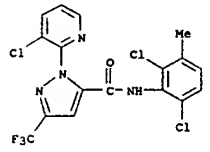


RN 636609-11-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2,6-dibromo-4-

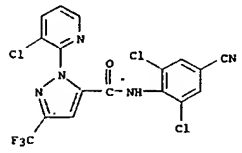
L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
nitrophenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 636609-17-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2,6-dichloro-3-methylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

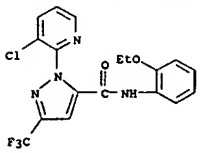


RN 636609-27-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2,6-dichloro-4-cyanophenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

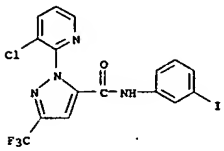


RN 636609-35-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2-ethoxyphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

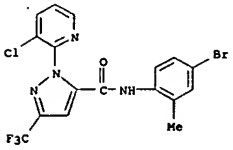
L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 636609-50-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(3-iodophenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

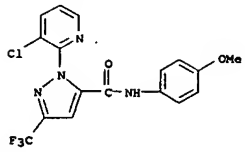


RN 636609-59-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-(4-bromo-2-methylphenyl)-1-(3-chloro-2-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 636609-70-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(4-methoxyphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 636609-89-7 CAPLUS
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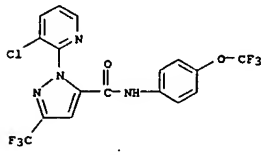
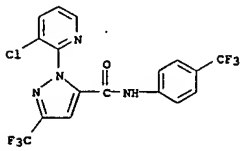


RN 636609-95-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-3-(trifluoromethyl)-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:844982 CAPLUS
DOCUMENT NUMBER: 140:59557
TITLE: Discovery of 1-(2-Aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl)]-4-yl]-1H-pyrazole-5-carboxamide (DPC602), a Potent, Selective, and Orally Bioavailable Factor Xa Inhibitor
AUTHOR(S): Pruitt, James R.; Pinto, Donald J. P.; Galemmo, Robert A., Jr.; Alexander, Richard S.; Rossi, Karen A.; Wells, Brian L.; Drummond, Spencer; Bostrom, Lori L.; Burdick, Debra; Bruckner, Robert; Chen, Haiying; Smallwood, Angela; Wong, Pancras C.; Wright, Matthew R.; Bai, Steven; Luettgen, Joseph M.; Knabb, Robert M.; Lam, Patrick Y. S.; Wexler, Ruth R.
CORPORATE SOURCE: Pharmaceutical Research Institute, Bristol-Myers Squibb Company, Pennington, NJ, 08534, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(25), 5298-5315
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:59557

AB Factor Xa, a serine protease, is at the critical juncture between the intrinsic and extrinsic pathways of the coagulation cascade. Inhibition of factor Xa has the potential to provide effective treatment for both venous and arterial thrombosis. The authors recently described a series of meta-substituted phenylpyrazoles that are highly potent, selective, and orally bioavailable factor Xa inhibitors. In this paper, the authors report their efforts to further optimize the selectivity profile of the factor Xa inhibitors with a series of ortho- and/or para-substituted phenylpyrazole derivs. The most potent compds. display sub-nanomolar inhibition consts. for factor Xa and show greater than 1000-fold selectivity against other serine proteases. These compds. are also effective in a rabbit model of arteriovenous shunt thrombosis. Optimization of this series led to the preclin. development of DPC602, a 2-(aminomethyl)phenylpyrazole analog, as a highly potent, selective, and orally bioavailable factor Xa inhibitor.

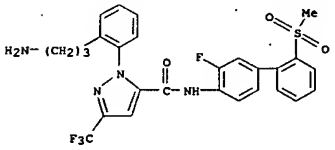
IT 637319-21-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of 1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl)]-4-yl]-1H-pyrazole-5-carboxamide and related compds. as orally bioavailable factor Xa inhibitors)

RN 637319-21-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(3-aminopropyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 875139-45-0
CMF C27 H24 F4 N4 O3 S

L3 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

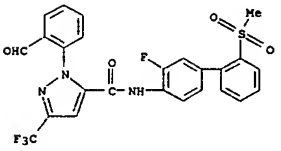


CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 637319-11-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl)]-4-yl]-1H-pyrazole-5-carboxamide and related compds. as orally bioavailable factor Xa inhibitors)

RN 637319-11-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-(2-formylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

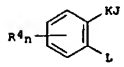


REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:261572 CAPLUS
DOCUMENT NUMBER: 138:267208
TITLE: Insecticidal compositions containing diamides
INVENTOR(S): Lahm, George Philip; Selby, Thomas Paul
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 246 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003026415 | A2 | 20030403 | WO 2002-US29468 | 20020917 |
| WO 2003026415 | A3 | 20031030 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1427705 | A2 | 20040616 | EP 2002-799589 | 20020917 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| BR 2002012799 | A | 20040803 | BR 2002-12799 | 20020917 |
| CN 1555364 | A | 20041215 | CN 2002-818247 | 20020917 |
| JP 2005504084 | T | 20050210 | JP 2003-530071 | 20020917 |
| US 2004235959 | A1 | 20041125 | US 2004-485096 | 20040126 |
| PRIORITY APPLN. INFO.: | | | US 2001-324083P | P 20010921 |
| | | | WO 2002-US29468 | W 20020917 |

OTHER SOURCE(S): MARPAT 138:267208
GI



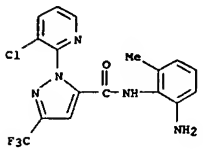
AB Compns. for controlling an invertebrate pest comprise a biol. effective amount of a compound I (Markush included), including all geometric and stereoisomers, N-oxides and agriculturally suitable salts thereof, and may optionally comprise addnl. components selected from the group consisting

L3 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:154424 CAPLUS
DOCUMENT NUMBER: 138:205057
TITLE: Preparation of N-[2-(heteroaryl)phenyl] pyrazole-5-carboxamides for controlling invertebrate pests
INVENTOR(S): Clark, David Alan; Finkelstein, Bruce Lawrence; Lahm, George Philip; Selby, Tom Paul; Stevenson, Thomas Martin
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 172 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

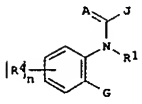
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003016304 | A1 | 20030227 | WO 2002-US26968 | 20020812 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1417204 | A1 | 20040512 | EP 2002-768688 | 20020812 |
| EP 1417204 | B1 | 20060118 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| BR 2002012186 | A | 20041005 | BR 2002-12186 | 20020812 |
| CN 1543460 | A | 20041103 | CN 2002-815961 | 20020812 |
| JP 2005502661 | T | 20050127 | JP 2003-521227 | 20020812 |
| AT 316085 | T | 20060215 | AT 2002-768688 | 20020812 |
| ES 2255624 | T3 | 20060701 | ES 2002-2768688 | 20020812 |
| US 2004242645 | A1 | 20041202 | US 2004-483117 | 20040609 |
| PRIORITY APPLN. INFO.: | | | US 2001-312440P | P 20010815 |
| | | | WO 2002-US26968 | W 20020812 |

OTHER SOURCE(S): MARPAT 138:205057
GI

L3 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
of surfactants, solid diluents and liq. diluents, and addnl. biol. active compds. or agents selected from the group consisting of pyrethroids, carbamates, neonicotinoids, neuronal sodium channel blockers, insecticidal macrocyclic lactones, γ-aminobutyric acid (GABA) antagonists, insecticidal ureas, juvenile hormone mimics, and biol. agents. such as Bacillus thuringiensis , Bt delta endotoxins, baculoviruses, entomopathogenic bacteria, viruses and fungi.
IT 503548-32-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diamides as insecticide)
RN 503548-32-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-(2-amino-6-methylphenyl)-1-(3-chloro-2-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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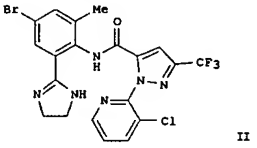
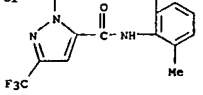


II

AB The title compds. [I; A = O, S; G = (un)substituted 5-6 membered heteroarom. ring or a 5-6 membered nonarom. heterocyclic ring optionally including one or two ring members selected from the group consisting of CO, SO or SO2; J = (un)substituted Ph, a 5-6 membered heteroarom. ring or an aromatic 8-10 membered fused carbobicyclic or heterobicyclic ring system; R1 = H, alkyl, alkenyl, etc.; R4 = alkyl, alkenyl, cycloalkyl, etc.; n = 1-4], useful for controlling an invertebrate pest, were prepared Thus, treating 1-(3-chloro-2-pyridinyl)-3-trifluoromethyl-1H-pyrazole-5-carboxylic acid with (COCl)2 in CH2Cl2 followed by addition of a solution of 4-bromo-2-(4,5-dihydro-1H-imidazol-2-yl)-6-methylbenzenamine (3-step preparation given), DMAP and Et3N in CH2Cl2 afforded II which provided excellent levels of plant protection (20% or less feeding damage) when tested at 50 ppm.
IT 500100-88-9P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of N-[2-(heteroaryl)phenyl] pyrazole-5-carboxamides for controlling invertebrate pests)
RN 500100-88-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2-(1H-imidazol-2-yl)-6-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 48.37 | 49.03 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -7.02 | -7.02 |

FILE 'REGISTRY' ENTERED AT 07:51:35 ON 08 JAN 2007


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2
DICTIONARY FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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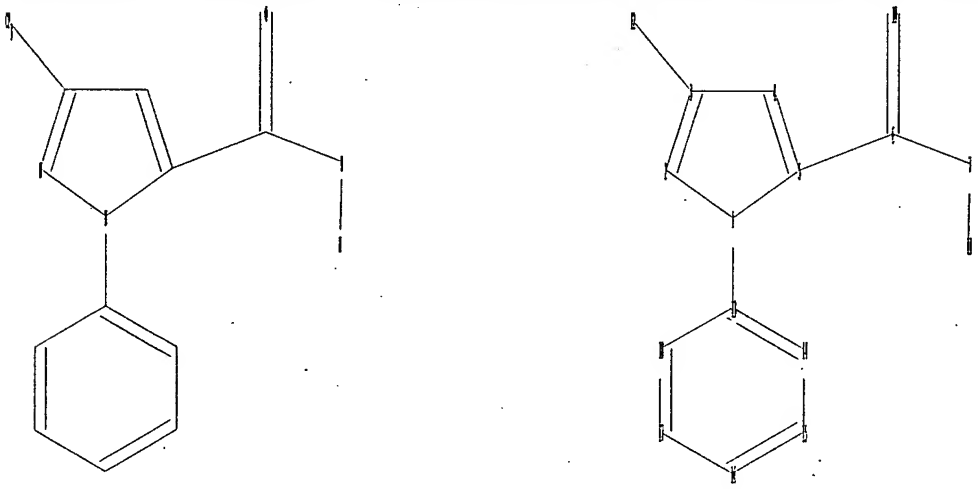
Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 5.str



chain nodes :
6 7 10 11 12

ring nodes :
1 2 3 4 5 13 14 15 16 17 18
chain bonds :
1-13 3-12 5-6 6-7 6-10 7-11
ring bonds :
1-5 1-2 2-3 3-4 4-5 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
1-5 1-2 1-13 2-3 3-4 4-5 6-7 6-10
exact bonds :
3-12 5-6 7-11
normalized bonds :
13-14 13-18 14-15 15-16 16-17 17-18

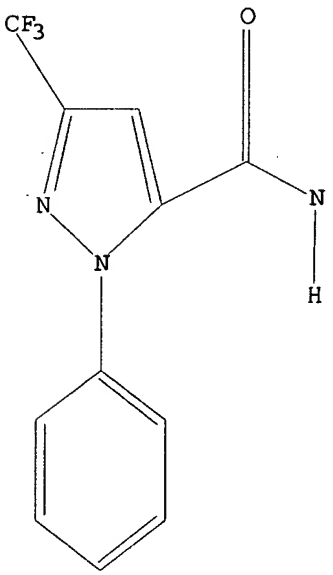
G1:Cb,Cy,Hy

G2:S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 10:CLASS 11:CLASS
12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom

L4 STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4 STR




G1 Cb,Cy,Hy
G2 S,N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 07:52:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      132 TO ITERATE

100.0% PROCESSED      132 ITERATIONS                          50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

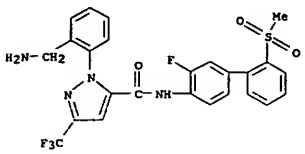
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1951 TO   3329
PROJECTED ANSWERS:             752 TO     1688

L5           50 SEA SSS SAM L4

=> d scan
```

L5 50 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI)
MF C25 H20 F4 N4 O3 S . C2 H F3 O2

CM 1



CM 2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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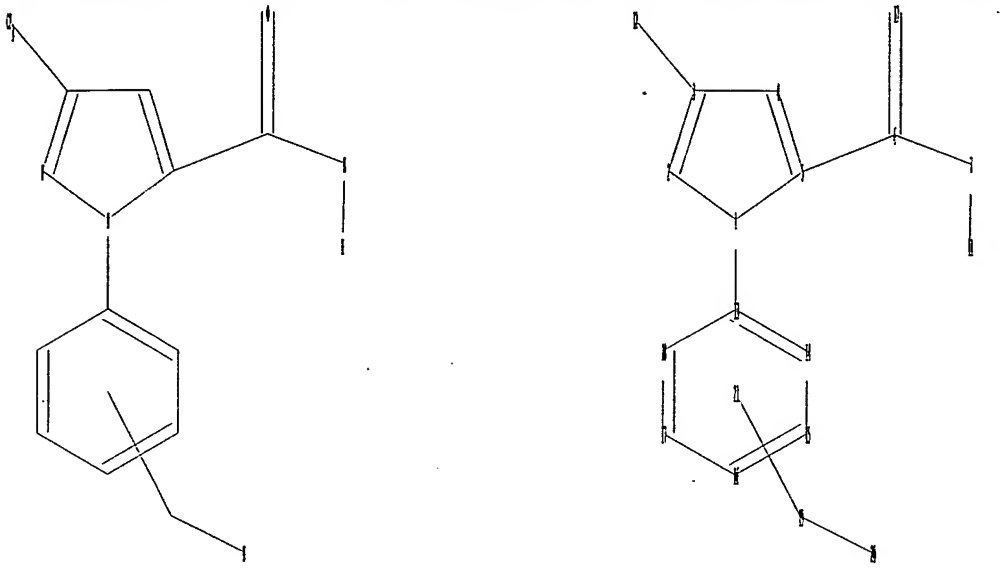


chain nodes :
6 7 10 11 12 19 20
ring nodes :
1 2 3 4 5 13 14 15 16 17 18
chain bonds :
1-13 3-12 5-6 6-7 6-10 7-11 19-20
ring bonds :
1-5 1-2 2-3 3-4 4-5 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
1-5 1-2 1-13 2-3 3-4 4-5 6-7 6-10 19-20
exact bonds :
3-12 5-6 7-11
normalized bonds :
13-14 13-18 14-15 15-16 16-17 17-18

G1:Cb,Cy,Hy

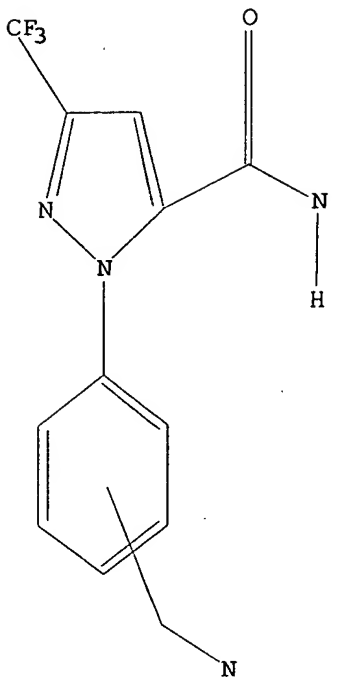
G2:S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 10:CLASS 11:CLASS
12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:Atom

L6 STRUCTURE UPLOADED

=> d
L6 HAS NO ANSWERS
L6 STR

10519356a.trn



G1 Cb,Cy,Hy

G2 S,N

Structure attributes must be viewed using STN Express query preparation.

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=> l6
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SAMPLE SCREEN SEARCH COMPLETED -      132 TO ITERATE

100.0% PROCESSED      132 ITERATIONS                          22 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1951 TO     3329
PROJECTED ANSWERS:             159 TO      721

L7            22 SEA SSS SAM L6

=> l6 full
FULL SEARCH INITIATED 07:56:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2606 TO ITERATE

100.0% PROCESSED     2606 ITERATIONS                         426 ANSWERS
SEARCH TIME: 00.00.01

L8           426 SEA SSS FUL L6
```

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   175.25     224.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -7.02

FILE 'MEDLINE' ENTERED AT 07:56:10 ON 08 JAN 2007

FILE 'CAPLUS' ENTERED AT 07:56:10 ON 08 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

=> l8
L9          36 L8

=> d ibib abs hitstr 1-36
```

L9 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1096816 CAPLUS
DOCUMENT NUMBER: 145:443880
TITLE: Odiparcil and a factor Xa inhibitor formulations for treatment of thromboembolic disorders
INVENTOR(S): Ohlstein, Eliot H.
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 42pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2006110726 | A2 | 20061019 | WO 2006-US13448 | 20060411 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-669985P P 20050411

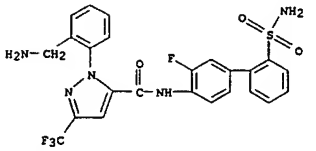
OTHER SOURCE(S): MARPAT 145:443880

AB The present invention relates to combinations of 4-methyl-2-oxo-2H-1-benzopyran-7-yl-5-thio-β-D-xylopyranoside (odiparcil)and factor Xa inhibitors, methods for producing the combinations, and methods of using the combinations for the treatment and prevention of various thromboembolic disorders in mammals, particularly humans. Thus, 2 parts odiparcil are combined with 1 part by weight rivaroxaban. The combined powders are then optionally milled to desired particle size range. The combination of the 2 drugs is then further combined with a wetting agent, disintegrant and/or filler and compressed into tablets of the following strengths: 50 mg odiparcil/25 mg rivaroxaban; 100 mg odiparcil/50 mg rivaroxaban; 200 mg odiparcil/100 mg rivaroxaban; 250 mg odiparcil/125 mg rivaroxaban.

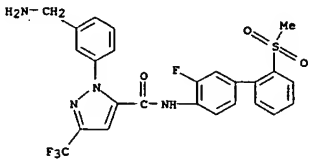
IT 228258-45-5, DPC 602 292135-59-2, DPC 423
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(odiparcil and factor Xa inhibitor formulations for treatment of thromboembolic disorders)

RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-(3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



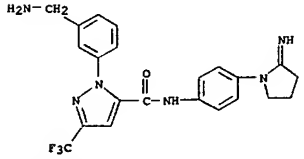
● HCl

L9 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1061760 CAPLUS
TITLE: Design and Evaluation of a Novel Class-Directed 2D Fingerprint to Search for Structurally Diverse Active Compounds
AUTHOR(S): Eckert, Hanna; Bajorath, Juergen
CORPORATE SOURCE: Department of Life Science Informatics, B-IT, Rheinische Friedrich-Wilhelms-Universitaet, Bonn, D-53113, Germany
SOURCE: Journal of Chemical Information and Modeling (2006), 46(6), 2515-2526
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Recent attempts to increase similarity search performance using mol. fingerprints have mostly focused on the evaluation of alternative similarity metrics or scoring schemes, rather than the development of new types of fingerprints. Here, the authors introduce a novel 2D fingerprint design (property descriptor value range-derived fingerprint or PDR-FP) that involves activity-oriented selection of property descriptors and the transformation of descriptor value ranges into a binary format such that each fingerprint bit position represents a specific value interval. The design is tailored toward multiple-template similarity searching and permits training on specific activity classes. In search calcns. on 15 compound classes of increasing structural diversity, the PDR fingerprint performed better than other state-of-the-art 2D fingerprints. Among the structurally diverse classes were six compound sets with peptide character, which represent a notoriously difficult chemotype for 2D similarity searching. In these cases, PDR-FP produced promising results, whereas other fingerprint methods mostly failed. PDR-FP is specifically designed for search calcns. on structurally diverse compds., and these calcns. are not influenced by mol. size effects, which represent a general problem for similarity searching using bit string representations.

IT 774536-86-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PRP (Properties); USES (Uses)
(design and evaluation of a class-directed 2D fingerprint to search for structurally diverse active compds.)

RN 774536-86-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

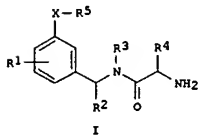
L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:635022 CAPLUS
DOCUMENT NUMBER: 145:103950
TITLE: Preparation of amino acid derivatives as inhibitors of protein arginine methyl transferases
INVENTOR(S): Purandare, Ashok Vinayak; Chen, Zhong
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 125 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2006069155 | A2 | 20060629 | WO 2005-US46362 | 20051221 |
| WO 2006069155 | A3 | 20061123 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-637893P P 20041221

OTHER SOURCE(S): MARPAT 145:103950
GI



I

AB The invention relates to compds. I [X is Ph or 5-membered heteroaryl; R1 is H, halogen, CN, alkyl or substituted alkyl, alkoxy, alkylthio, or alkylsulfonyl; R2 is H or alkyl; R3 is H, Me, or Et; R4 is H, Me, Et, iso-Pr, CH2Ph, OH, or OPh; or R3 and R4 may form a 5- or 6-membered heterocycle; R5 is -W-(CH2)0-3-O0-1-R6, where W is CONH, 1,3,4-oxadiazole-2,5-diyl, etc and R6 is (un)substituted cycloalkyl, heterocyclyl, or aryl] or a stereoisomer, tautomer, or pharmaceutically-acceptable salt and their use in the treatment of hyperproliferative, inflammatory, infectious, and immunoregulatory disorders and diseases. Thus, I [R1-R3 = H, R4 = Me, R5-X = 5-(benzylcarbamoyl)-3-(trifluoromethyl)-1-pyrazolyl] was prepd. from 1-(3-cyanophenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxylic acid by hydrogenation over Pd/C, followed by amidation reactions with Boc-Ala-OSu and benzylamine. The product was assayed for inhibition of tumor cell proliferation using the 3H thymidine incorporation protocol (IC50 < 10 μM).

IT 895522-42-6P 895522-43-7P 895522-44-8P
895522-45-9P 895522-46-0P 895522-47-1P
895522-49-3P 895522-51-7P 895522-56-2P
895522-57-3P 895522-58-4P 895522-59-5P
895522-60-8P 895522-61-9P 895522-62-0P
895522-63-1P 895522-64-2P 895522-65-3P
895522-66-4P 895522-67-5P 895522-68-6P
895522-69-7P 895522-70-0P 895522-71-1P
895522-72-2P 895522-73-3P 895522-74-4P
895522-75-5P 895522-76-6P 895522-77-7P
895522-78-8P 895522-79-9P 895522-80-2P
895522-81-3P 895522-82-4P 895522-83-5P
895522-84-6P 895522-85-7P 895522-86-8P
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895522-93-7P 895522-94-8P 895522-95-9P
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895523-05-4P 895523-06-5P 895523-07-6P
895523-08-7P 895523-09-8P 895523-10-1P
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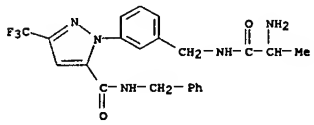
895523-17-8P 895523-18-9P 895523-19-0P
895523-20-3P 895523-21-4P 895523-22-5P
895523-23-6P 895523-24-7P 895523-25-8P
895523-26-9P 895523-27-0P 895523-28-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid derivs. as inhibitors of protein arginine Me transferases)

RN 895522-42-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(phenylmethyl)-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 895522-41-5

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C22 H22 F3 N5 O2

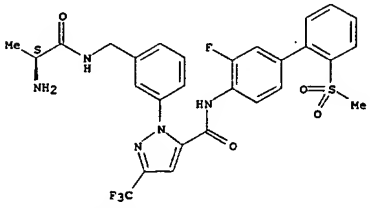


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 895522-43-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

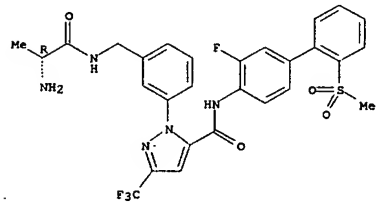
Absolute stereochemistry.



RN 895522-44-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2R)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

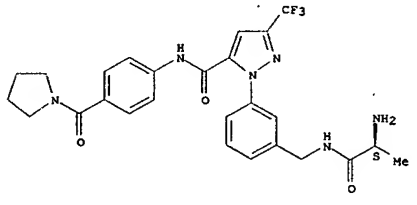
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-45-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

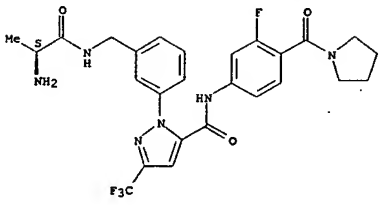
Absolute stereochemistry.



RN 895522-46-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

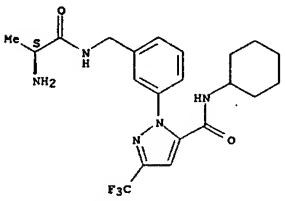
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-cyclohexyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

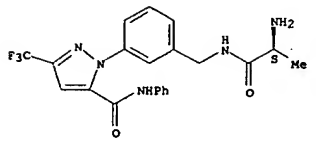
Absolute stereochemistry.



RN 895522-49-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-phenyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

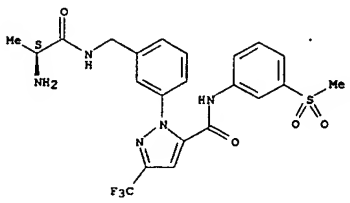
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



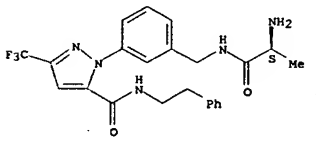
RN 895522-51-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[3-(methylsulfonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 895522-56-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(2-phenylethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

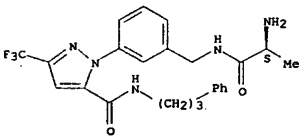
Absolute stereochemistry.



L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

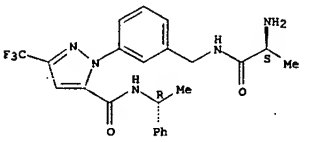
RN 895522-57-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-phenylpropyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



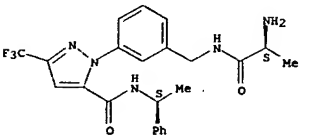
RN 895522-58-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1R)-1-phenylethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 895522-59-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1S)-1-phenylethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

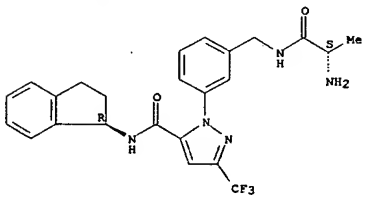
Absolute stereochemistry.



L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

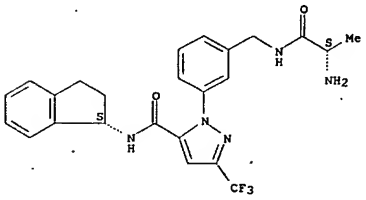
RN 895522-60-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1R)-2,3-dihydro-1H-inden-1-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 895522-61-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1S)-2,3-dihydro-1H-inden-1-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

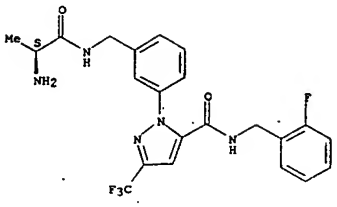
Absolute stereochemistry.



RN 895522-62-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-fluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

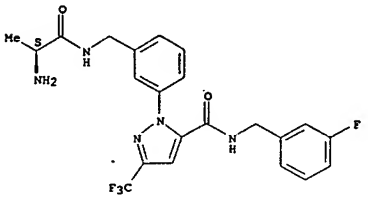
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-63-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3-fluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

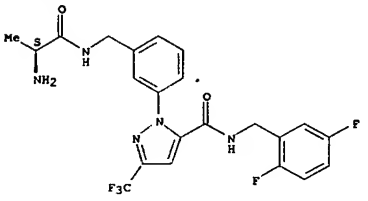
Absolute stereochemistry.



RN 895522-64-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-fluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

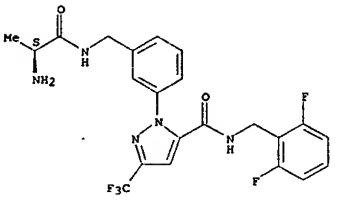
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-67-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2,6-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

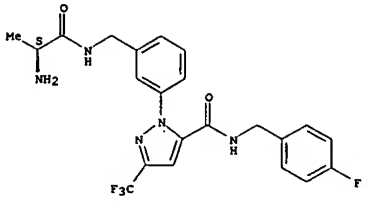
Absolute stereochemistry.



RN 895522-68-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3,4-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

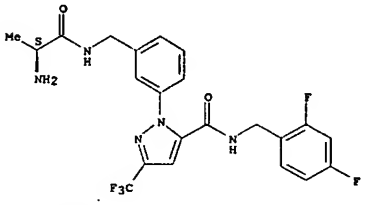
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-65-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2,4-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

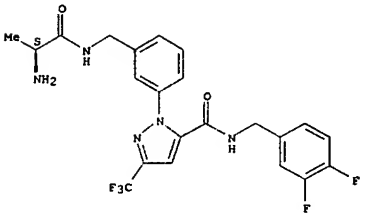
Absolute stereochemistry.



RN 895522-66-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2,5-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

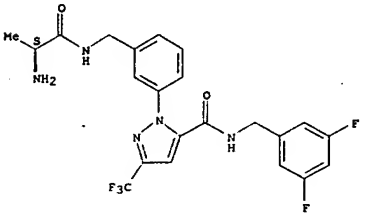
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-69-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3,5-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

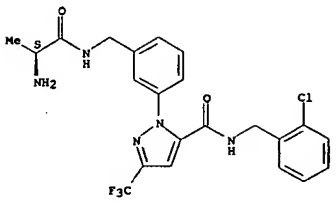
Absolute stereochemistry.



RN 895522-70-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-chlorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

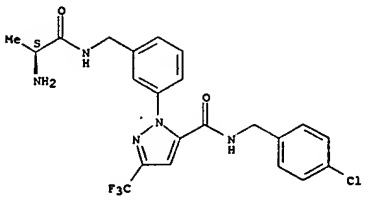
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-71-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-chlorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

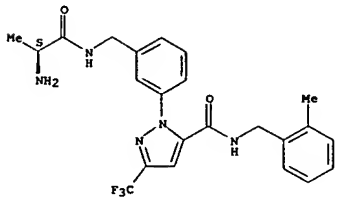
Absolute stereochemistry.



RN 895522-72-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-methylphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

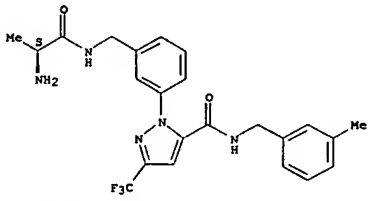
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-73-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3-methylphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

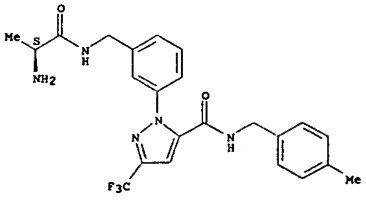
Absolute stereochemistry.



RN 895522-74-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-methylphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

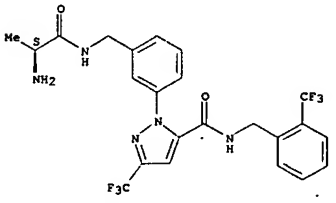
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-75-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-N-[[2-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

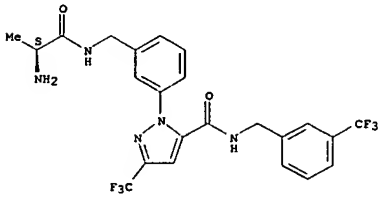
Absolute stereochemistry.



RN 895522-76-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-N-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

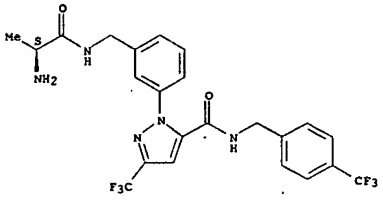
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-77-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

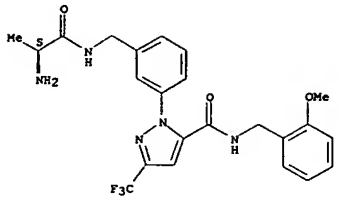
Absolute stereochemistry.



RN 895522-78-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-methoxyphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

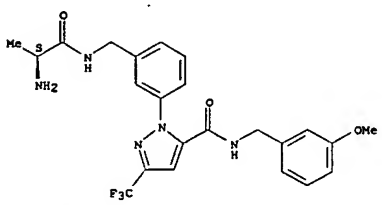
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-79-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3-methoxyphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

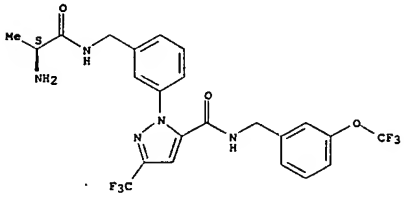
Absolute stereochemistry.



RN 895522-80-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-methoxyphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

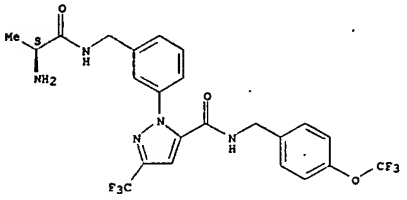
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-83-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[4-(trifluoromethoxy)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

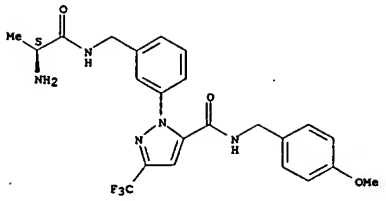
Absolute stereochemistry.



RN 895522-84-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-([1,1'-biphenyl]-3-ylmethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

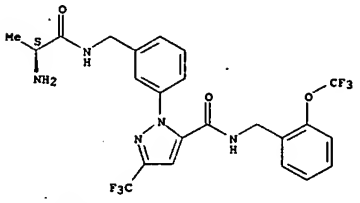
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-81-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[2-(trifluoromethoxy)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

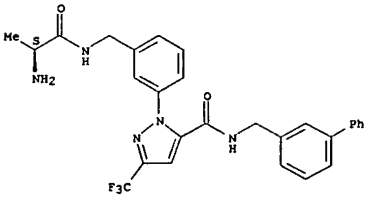
Absolute stereochemistry.



RN 895522-82-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[3-(trifluoromethoxy)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

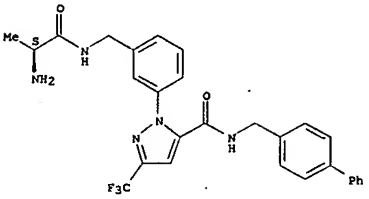
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-85-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-([1,1'-biphenyl]-4-ylmethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

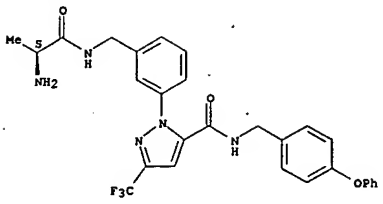
Absolute stereochemistry.



RN 895522-86-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-phenoxyphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

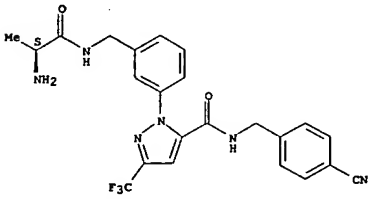
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-87-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-cyanophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

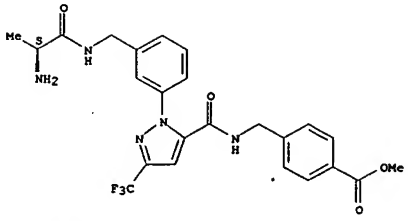
Absolute stereochemistry.



RN 895522-88-0 CAPLUS
CN Benzoic acid, 4-[[[[1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

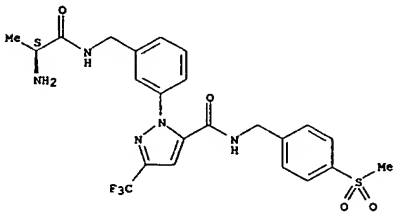
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-89-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[4-(methylsulfonyl)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

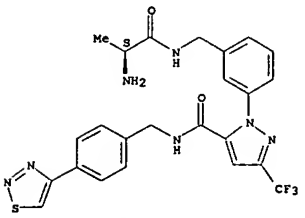
Absolute stereochemistry.



RN 895522-90-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[4-(1,2,3-thiadiazol-4-yl)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

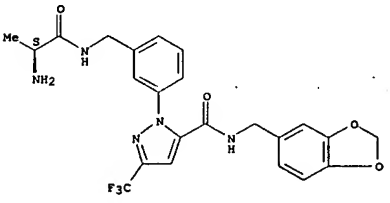
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-91-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1,3-benzodioxol-5-ylmethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

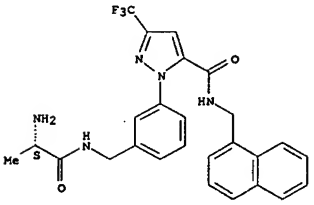
Absolute stereochemistry.



RN 895522-92-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1-naphthalenylmethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

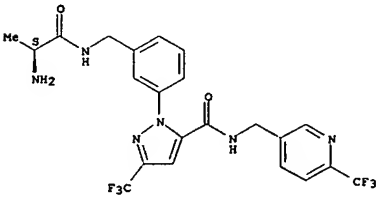
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-93-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-N-[[6-(trifluoromethyl)-3-pyridinyl]methyl]- (9CI) (CA INDEX NAME)

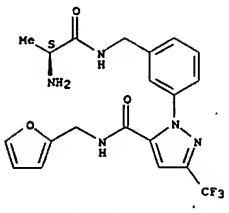
Absolute stereochemistry.



RN 895522-94-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(2-furanylmethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

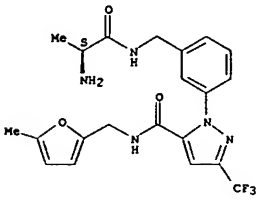
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-95-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(5-methyl-2-furanyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

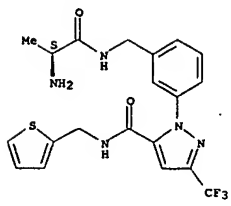
Absolute stereochemistry.



RN 895522-96-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(2-thienylmethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

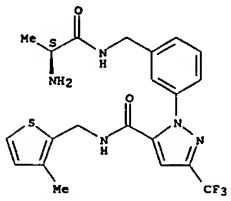
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-97-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3-methyl-2-thienyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

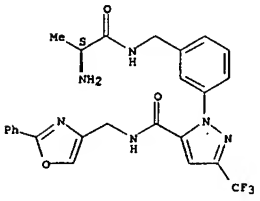
Absolute stereochemistry.



RN 895522-98-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-phenyl-4-oxazolyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

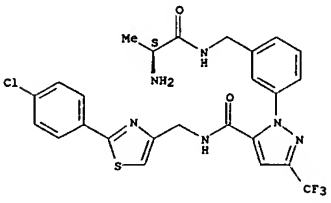
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-99-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-(4-chlorophenyl)-4-thiazolyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

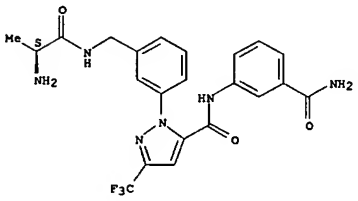
Absolute stereochemistry.



RN 895523-00-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-(aminocarbonyl)phenyl]-1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

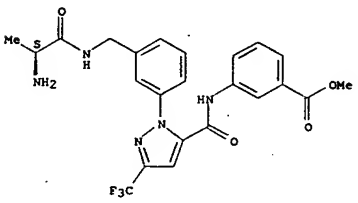
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-01-0 CAPLUS
CN Benzoic acid, 3-[[[1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

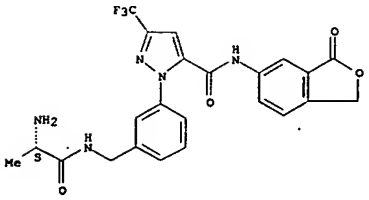
Absolute stereochemistry.



RN 895523-02-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1,3-dihydro-3-oxo-5-isobenzofuranyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

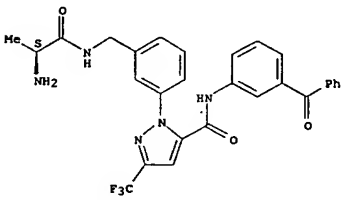
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-03-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-benzoylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

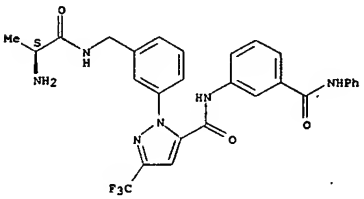
Absolute stereochemistry.



RN 895523-04-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[3-[(methylamino)carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

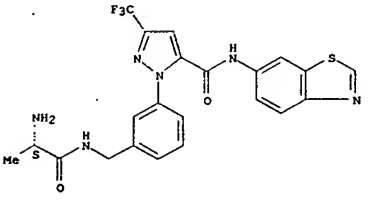
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-07-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-6-benzothiazolyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

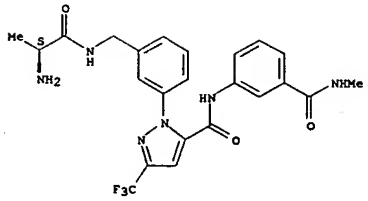
Absolute stereochemistry.



RN 895523-08-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(2-methyl-5-benzothiazolyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

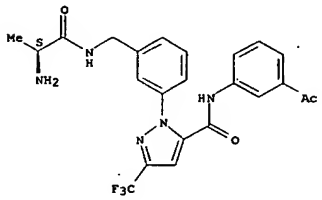
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-05-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-(3-acetylphenyl)-1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

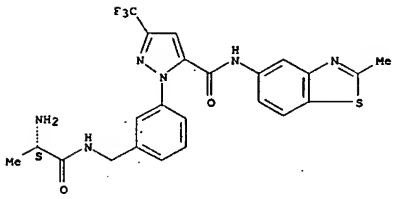
Absolute stereochemistry.



RN 895523-06-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[3-[(phenylamino)carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

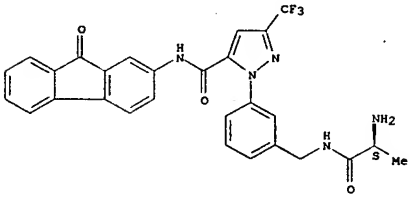
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-09-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(9-oxo-9H-fluoren-2-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

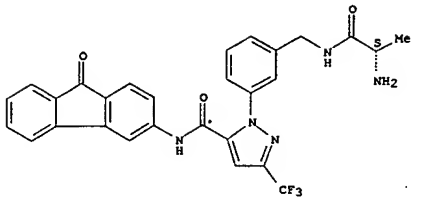
Absolute stereochemistry.



RN 895523-10-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(9-oxo-9H-fluoren-3-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

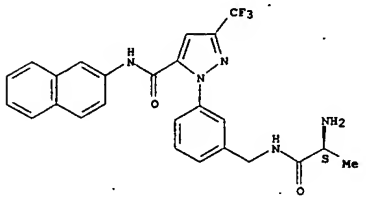
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-11-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-2-naphthalenyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

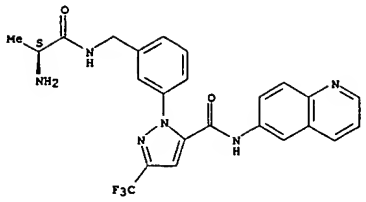
Absolute stereochemistry.



RN 895523-12-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-6-quinolinyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

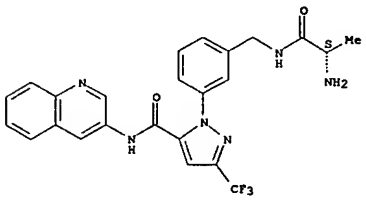
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-13-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-3-quinolinyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

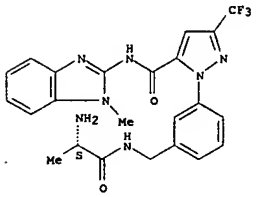
Absolute stereochemistry.



RN 895523-14-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1-methyl-1H-benzimidazol-2-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

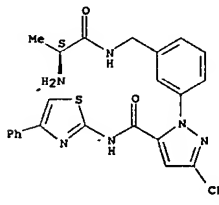
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-15-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(4-phenyl-2-thiazolyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

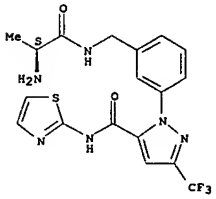
Absolute stereochemistry.



RN 895523-16-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-2-thiazolyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

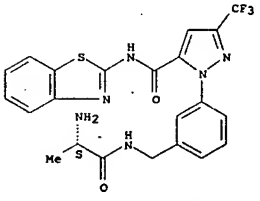
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-17-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-2-benzothiazolyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

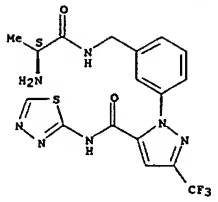
Absolute stereochemistry.



RN 895523-18-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-1,3,4-thiadiazol-2-yl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

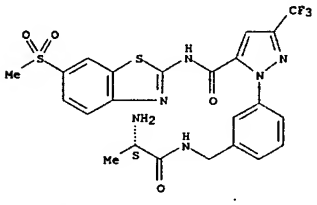
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-19-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[6-(methylsulfonyl)-2-benzothiazolyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

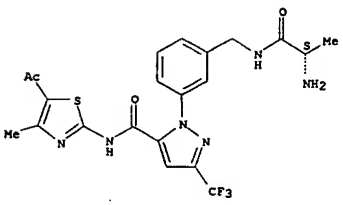
Absolute stereochemistry.



RN 895523-20-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-(5-acetyl-4-methyl-2-thiazolyl)-1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

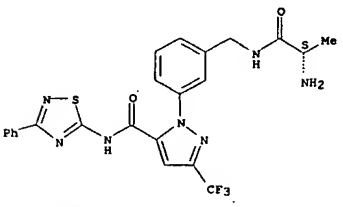
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-21-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-phenyl-1,2,4-thiadiazol-5-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

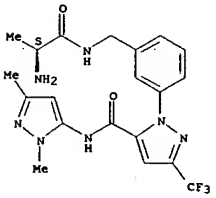
Absolute stereochemistry.



RN 895523-22-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1,3-dimethyl-1H-pyrazol-5-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

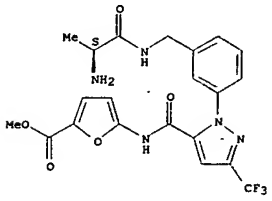
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-23-6 CAPLUS
CN 2-Furancarboxylic acid, 5-[[[1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

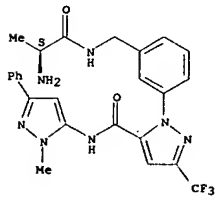
Absolute stereochemistry.



RN 895523-24-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1-methyl-3-phenyl-1H-pyrazol-5-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

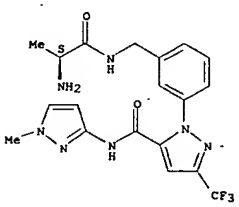
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-25-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1-methyl-1H-pyrazol-3-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

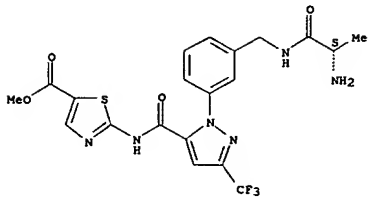
Absolute stereochemistry.



RN 895523-26-9 CAPLUS
CN 5-Thiazolecarboxylic acid, 2-[[[1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

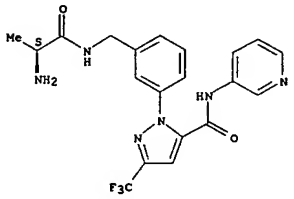
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-27-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-3-pyridinyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

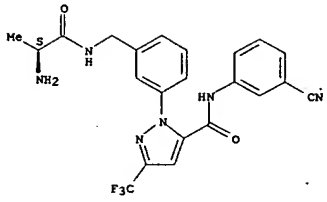
Absolute stereochemistry.



RN 895523-28-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-cyanophenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

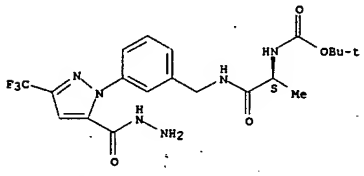
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 895524-51-3P 895524-53-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino acid derivs. as inhibitors of protein arginine Me
transferases)
RN 895524-51-3 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-[3-[[[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-, hydrazide (9CI) (CA INDEX NAME)

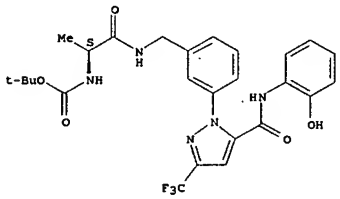
Absolute stereochemistry.



RN 895524-53-5 CAPLUS
CN Carbamic acid, [(1S)-2-[[[3-[5-[[(2-hydroxyphenyl)amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]amino]-1-methyl-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

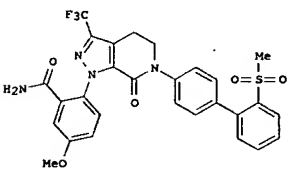
ACCESSION NUMBER: 2006:388784 CAPLUS
DOCUMENT NUMBER: 144:432799
TITLE: Preparation of pyrazolylbenzamides and pyrazolopyridinylbenzamides as factor Xa inhibitors for the treatment of thromboembolic disorders
INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Li, Renhua; Haque,
Tasir S.; Rossi, Karen A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 178 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 2006089496 | A1 | 20060427 | US 2005-256893 | 20051024 |
| WO 2006047528 | A2 | 20060504 | WO 2005-US38401 | 20051025 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-622236P P 20041026
US 2005-256893 A 20051024

OTHER SOURCE(S): MARPAT 144:432799
GI



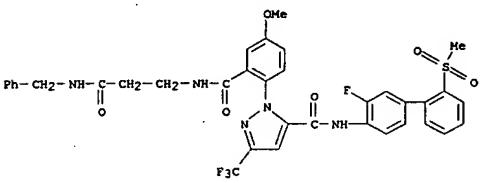
II

AB Title compds. and analogs I P4-P-M-M4 (wherein M = certain carbocycle or heterocycle; P (fused onto ring M) = certain carbocycle or heterocycle;

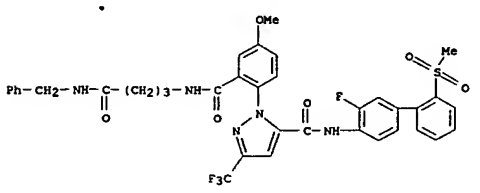
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
when P is absent P4 and M4 are directly attached to the 1,2, 1,3 and 1,4 positions of ring M; P4 = 2-(aminocarbonyl)phenyl, etc.; M4 = methylsulfonylbiphenyl, etc.], esp. pyrazolylbenzamides and pyrazolopyridinylbenzamides such as II, and stereoisomers, pharmaceutically acceptable salts or solvate forms thereof were prepd. as factor Xa inhibitors. A no. of the invented compds. were found to exhibit
Ki of ≤10 μM against purified human factor Xa. Therefore, I and their pharmaceutical compns. are useful for the treatment of thromboembolic disorders.

IT 885022-19-5P 885022-21-9P 885022-23-1P
885022-25-3P 885022-27-5P 885022-29-7P
885022-31-1P 885022-33-3P 885022-35-5P
885022-37-7P 885022-39-9P 885022-41-3P
885022-43-5P 885022-45-7P 885022-47-9P
885022-49-1P 885022-50-4P 885022-51-5P
885022-52-6P 885022-54-8P 885022-55-9P
885022-57-1P 885022-58-2P 885022-59-3P
885022-60-6P 885022-61-7P 885022-63-9P
885022-65-1P 885022-67-3P 885022-69-5P
885022-70-8P 885022-71-9P 885022-73-1P
885022-74-2P 885022-75-3P 885022-76-4P
885022-77-5P 885022-79-7P 885022-80-0P
885022-81-1P 885022-82-2P 885022-83-3P
885022-84-4P 885022-87-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrazolylbenzamides and pyrazolopyridinylbenzamides as factor Xa inhibitors for treatment of thromboembolic disorders)

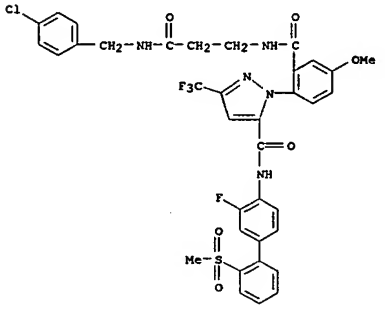
RN 885022-19-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[3-oxo-3-[(phenylmethyl)amino]propyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-21-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[4-oxo-4-[(phenylmethyl)amino]butyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

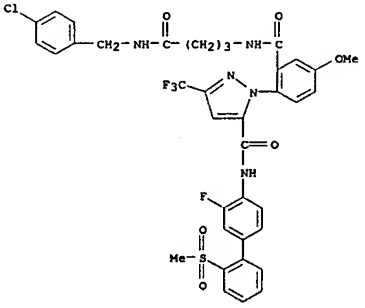


RN 885022-23-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[3-[[(4-chlorophenyl)methyl]amino]-3-oxopropyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-25-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[4-[[(4-chlorophenyl)methyl]amino]-4-oxobutyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

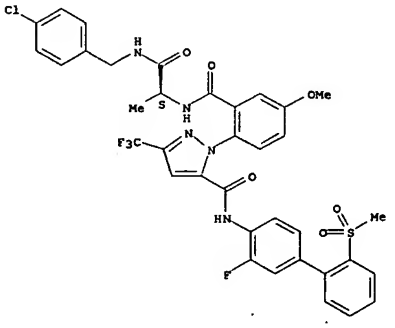
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-27-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-2-[[(4-chlorophenyl)methyl]amino]-1-methyl-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

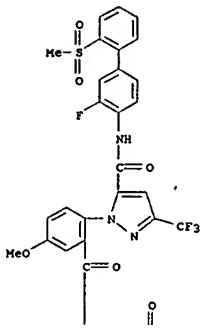
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



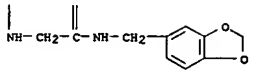
RN 885022-29-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[2-[(1,3-benzodioxol-5-ylmethyl)amino]-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



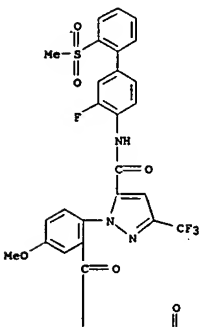
PAGE 2-A



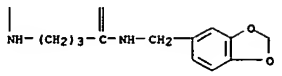
RN 885022-31-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[4-[(1,3-benzodioxol-5-ylmethyl)amino]-4-oxobutyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



PAGE 2-A

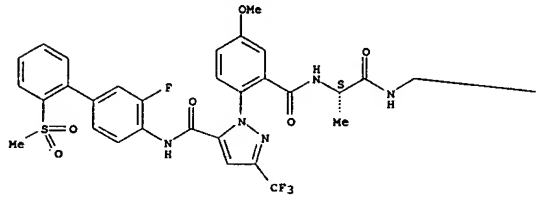


RN 885022-33-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-2-[(1,3-benzodioxol-5-ylmethyl)amino]-1-methyl-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI)
(CA INDEX NAME)

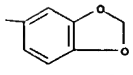
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



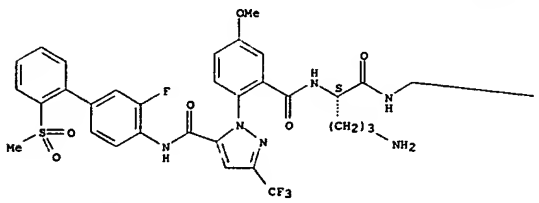
PAGE 1-B



RN 885022-35-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-4-amino-1-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]butyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

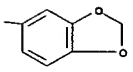
Absolute stereochemistry.

PAGE 1-A



L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

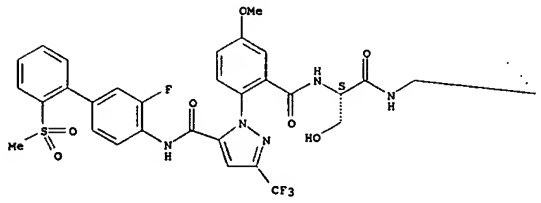
PAGE 1-B



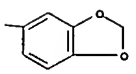
RN 885022-37-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-2-[(1,3-benzodioxol-5-ylmethyl)amino]-1-(hydroxymethyl)-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

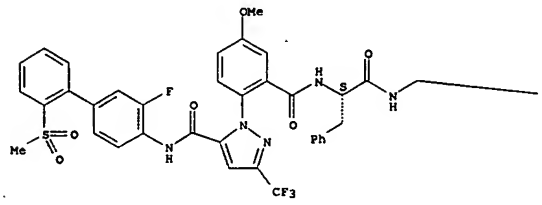


RN 885022-39-9 CAPLUS

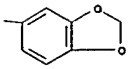
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-2-[(1,3-benzodioxol-5-ylmethyl)amino]-2-oxo-1-(phenylmethyl)ethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



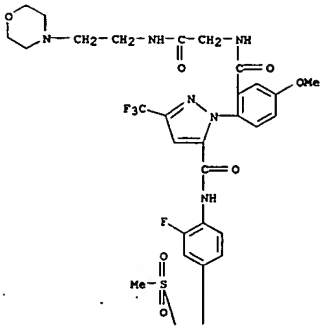
PAGE 1-B



RN 885022-41-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[2-[[2-(4-morpholinyl)ethyl]amino]-2-oxoethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A

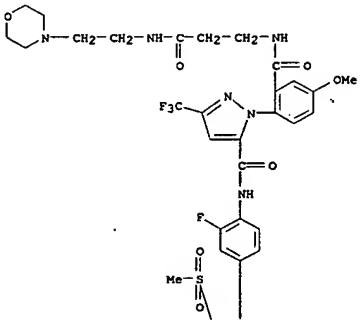


PAGE 2-A

RN 885022-43-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[3-[[2-(4-morpholinyl)ethyl]amino]-3-oxopropyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A

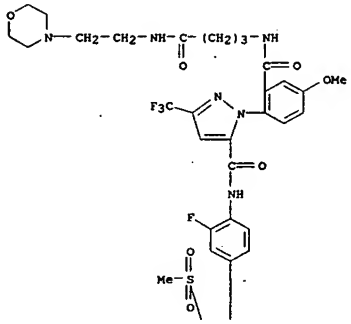


PAGE 2-A

RN 885022-45-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[4-[[2-(4-morpholinyl)ethyl]amino]-4-oxobutyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

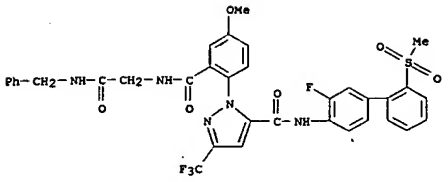
PAGE 1-A



PAGE 2-A

RN 885022-47-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[2-oxo-2-[(phenylmethyl)amino]ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

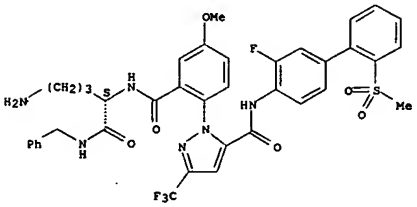
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-49-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-4-amino-1-

[[(phenylmethyl)amino]carbonyl]butyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI)
(CA INDEX NAME)

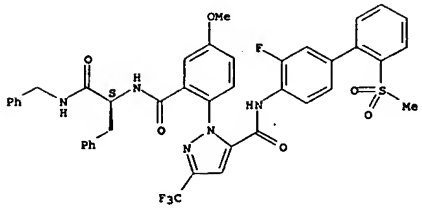
Absolute stereochemistry.



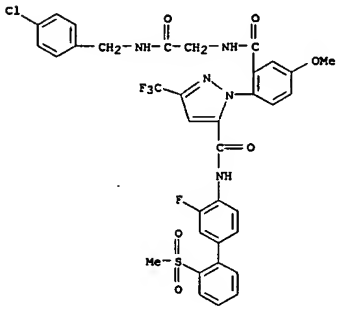
RN 885022-50-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[(1S)-2-oxo-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

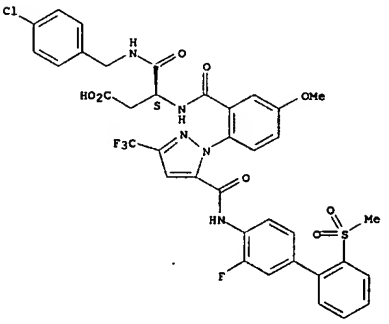


RN 885022-51-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[2-[[(4-chlorophenyl)methyl]amino]-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-52-6 CAPLUS
CN Butanoic acid, 4-[[(4-chlorophenyl)methyl]amino]-3-[[2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]-5-methoxybenzoyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry.

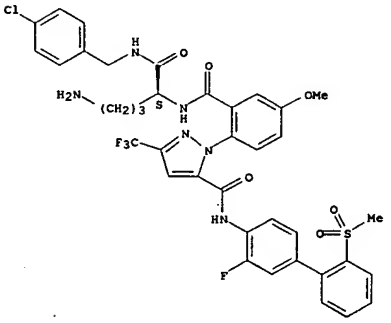


RN 885022-54-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-4-amino-1-[[[(4-

chlorophenyl)methyl]amino]carbonyl]butyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

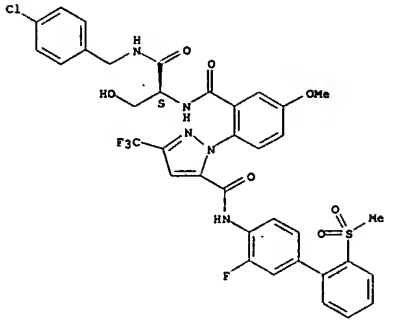


RN 885022-55-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-[[[(1S)-2-[[(4-chlorophenyl)methyl]amino]-

1-(hydroxymethyl)-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

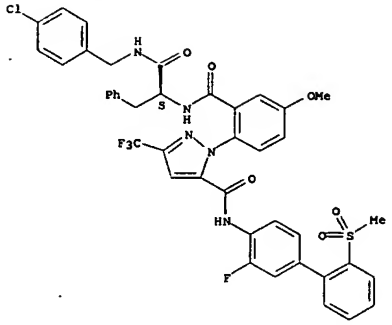
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-57-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-[[[(1S)-2-[[(4-chlorophenyl)methyl]amino]-
2-oxo-1-(phenylmethyl)ethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

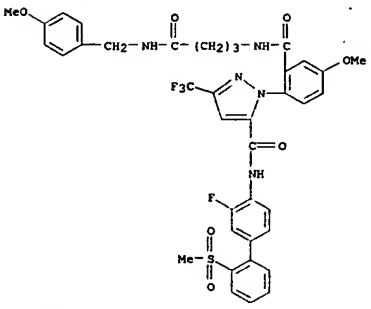
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

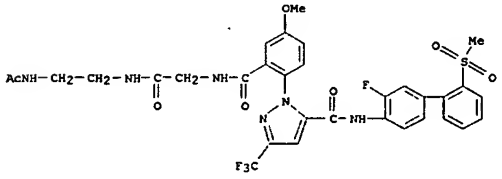


RN 885022-58-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[[[4-[[(4-methoxyphenyl)methyl]amino]-4-
oxobutyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX
NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



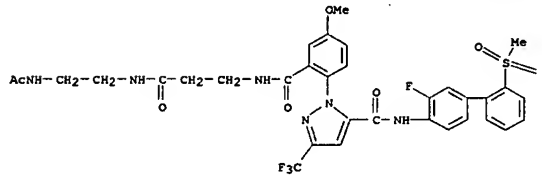
RN 885022-59-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[2-[(2-(acetylamino)ethyl]amino]-2-
oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)



RN 885022-60-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[3-[[2-(acetylamino)ethyl]amino]-3-
oxopropyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

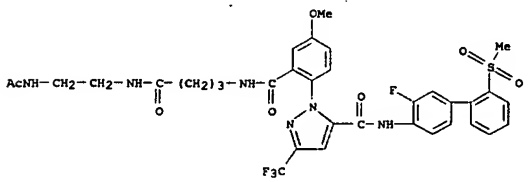
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



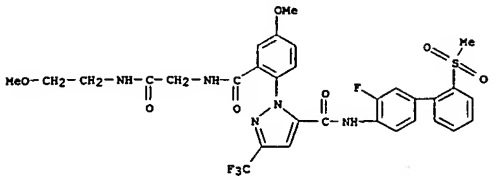
PAGE 1-B

RN 885022-61-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[4-[(2-(acetylamino)ethyl]amino]-4-
oxobutyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

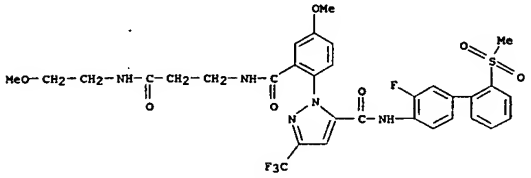


RN 885022-63-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[[[2-[(2-methoxyethyl)amino]-2-
oxoethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX
NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

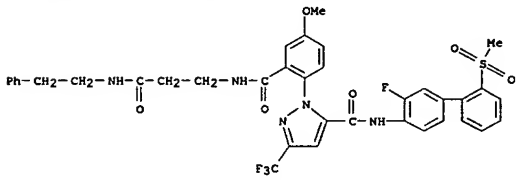


RN 885022-65-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[[[3-[(2-methoxyethyl)amino]-3-
oxopropyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



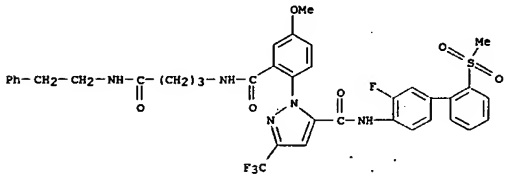
RN 885022-67-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[[[4-[(2-methoxyethyl)amino]-4-
oxobutyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-71-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-

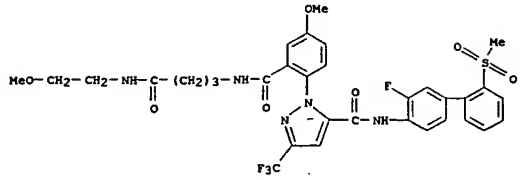
4-yl]-1-[4-methoxy-2-[[[4-oxo-4-[(2-phenylethyl)amino]butyl]amino]carbonyl
]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-73-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-4-amino-1-[[(2-
phenylethyl)amino]carbonyl]butyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-
fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-
(9CI)
(CA INDEX NAME)

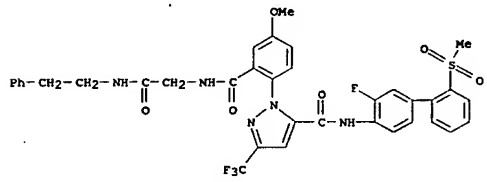
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-69-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-

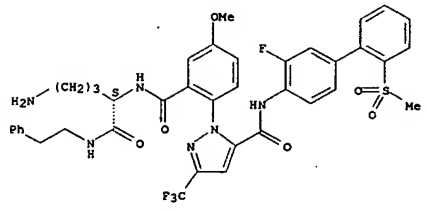
4-yl]-1-[4-methoxy-2-[[[2-oxo-2-[(2-phenylethyl)amino]ethyl]amino]carbonyl
]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-70-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-

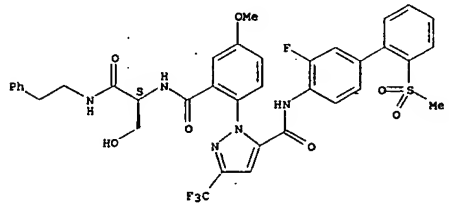
4-yl]-1-[4-methoxy-2-[[[3-oxo-3-[(2-phenylethyl)amino]propyl]amino]carbony
l]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-74-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[2-[[[(1S)-1-(hydroxymethyl)-2-oxo-2-[(2-
phenylethyl)amino]ethyl]amino]carbonyl]-4-methoxyphenyl]-3-
(trifluoromethyl)- (9CI) (CA INDEX NAME)

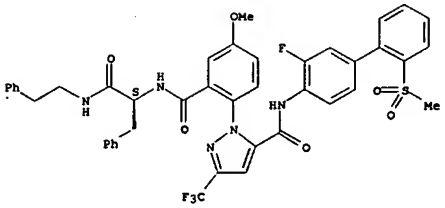
Absolute stereochemistry.



RN 885022-75-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[[[(1S)-2-oxo-2-[(2-phenylethyl)amino]-1-
(phenylmethyl)ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI)
(CA
INDEX NAME)

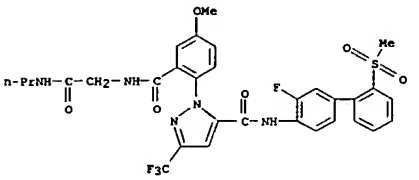
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-76-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-

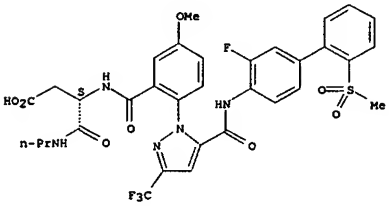
4-yl]-1-[4-methoxy-2-[[[2-oxo-2-(propylamino)ethyl]amino]carbonyl]phenyl]-
3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-77-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-

4-yl]-1-[4-methoxy-2-[[[3-oxo-3-(propylamino)propyl]amino]carbonyl]phenyl]-
3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

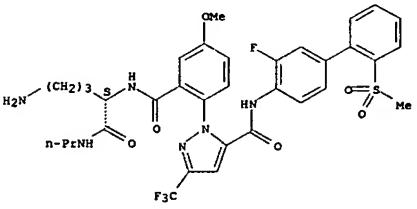
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-81-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-4-amino-1-

[(propylamino)carbonyl]butyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

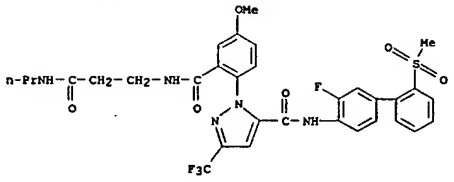


RN 885022-82-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-

4-yl]-1-[2-[[[(1S)-1-(hydroxymethyl)-2-oxo-2-(propylamino)ethyl]amino]carb
onyl]-4-methoxyphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

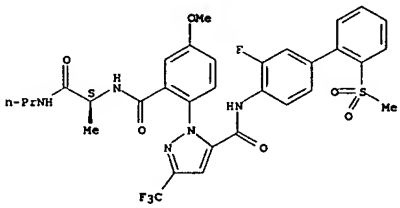
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-79-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[[[(1S)-1-methyl-2-oxo-2-
(propylamino)ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

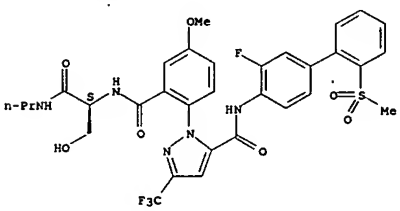
Absolute stereochemistry.



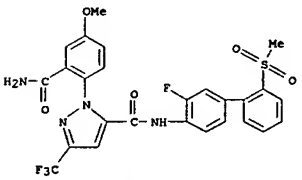
RN 885022-80-0 CAPLUS
CN Butanoic acid, 3-[[2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-
yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]-5-
methoxybenzoyl]amino]-4-oxo-4-(propylamino)-, (3S)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

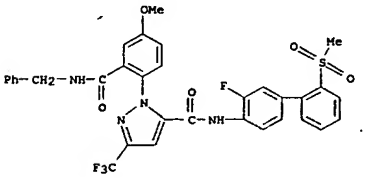
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-83-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminocarbonyl)-4-methoxyphenyl]-N-[3-
fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-
(9CI)
(CA INDEX NAME)

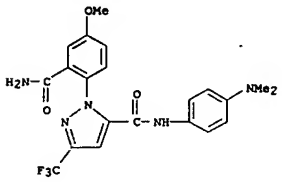


RN 885022-84-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[[(phenylmethyl)amino]carbonyl]phenyl]-3-
(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 885022-87-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminocarbonyl)-4-methoxyphenyl]-N-[4-(dimethylamino)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



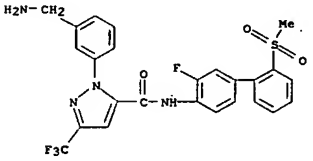
L9 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:188866 CAPLUS
DOCUMENT NUMBER: 144:362579
TITLE: Aminobenzisoxazoles with biaryl P4 moieties as potent,
selective, and orally bioavailable factor Xa inhibitors
AUTHOR(S): Quan, Mimi L.; Han, Qi; Fevig, John M.; Lam, Patrick Y. S.; Bai, Steve; Knabb, Robert M.; Luettgen, Joseph M.; Wong, Pancras C.; Wexler, Ruth R.
CORPORATE SOURCE: Discovery Chemistry, Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(7), 1795-1798
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:362579

AB We have previously reported on a series of aminobenzisoxazoles as potent, selective, and orally bioavailable factor Xa inhibitors, which culminated in the discovery of razaxaban. Herein, we describe another approach to improve factor Xa inhibitory potency and pharmacokinetic profile by incorporating basic and water soluble functionalities on the terminal ring of the P4 biaryl group found in our earlier Xa inhibitors. This approach resulted in a series of potent, selective, and orally bioavailable factor Xa inhibitors.

IT 292135-59-2, DPC423
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Aminobenzisoxazoles with biaryl P4 moieties as potent, selective, and orally bioavailable factor Xa inhibitors)

RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L9 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

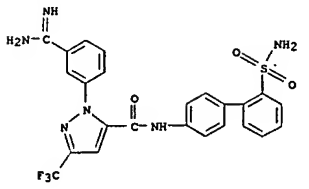
ACCESSION NUMBER: 2006:165187 CAPLUS
DOCUMENT NUMBER: 144:304521
TITLE: Comparative study of factor Xa inhibitors using molecular docking/SVM/HQSAR/3D-QSAR methods
AUTHOR(S): Sun, Jing; Chen, Hai Feng; Xia, Hai Rong; Yao, Jian Hua; Fan, Bo Tao
CORPORATE SOURCE: Laboratory of Computer Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: QSAR & Combinatorial Science (2006), 25(1), 25-45
CODEN: QCSSAU; ISSN: 1611-020X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding modes of a group of Factor Xa (fXa) inhibitors were studied using FlexX. CoMFA, CoMSIA, HQSAR and SVM models for inhibition potency were constructed with the conformers obtained from the mol. docking. 3D-QSAR models for oral bioavailability were also constructed with the subset inhibitors. The results show that these models possess good prediction ability. The influence of substituents for the activity and oral bioavailability were explored by comparing the constructed 3D-QSAR models. We found that some substituents have consistent effects on inhibition potency and oral bioavailability, but some have inconsistent effects. We observed equally that the different methods involved in this study, such as mol. docking, SVM, HQSAR and 3D-QSAR models, could be used not only for the prediction, but they are also complementary each to other. They are helpful for better understanding the interaction mechanism between inhibitors and fXa receptor.

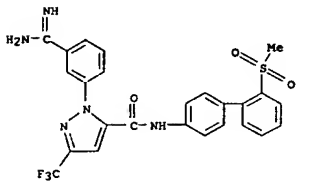
IT 209954-59-6 209954-94-9 209955-38-4
209955-48-6 209955-60-2 209957-33-5
209957-35-7 209957-47-1 228257-38-3
228257-44-1 228257-50-9 228257-56-5
228258-43-3 228258-44-4 228258-45-5
228258-46-6 875139-46-1 875139-51-8
875139-66-5 875139-67-6
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(comparative study of factor Xa inhibitors using mol. docking/SVM/HQSAR/QSAR methods)

RN 209954-59-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

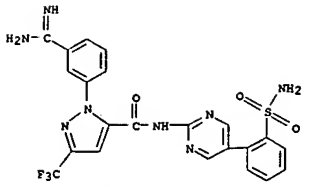


RN 209954-94-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

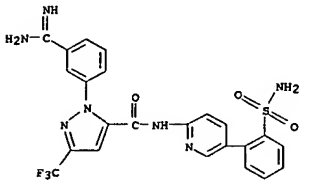


RN 209955-38-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

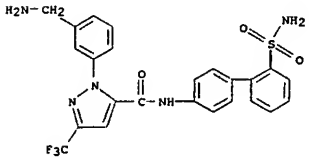


RN 209955-48-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

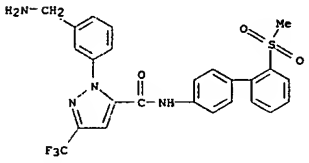


RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

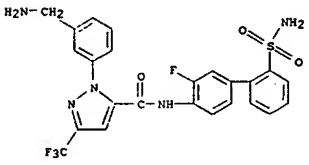
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-33-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

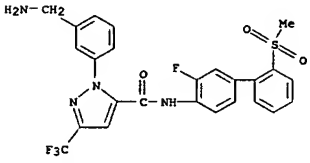


RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

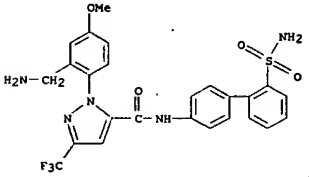


RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

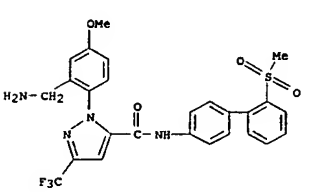
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228257-38-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

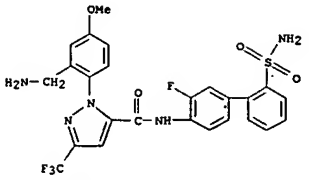


RN 228257-44-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

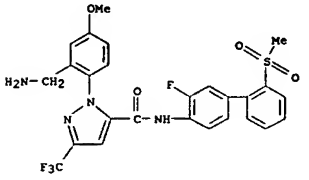


RN 228257-50-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

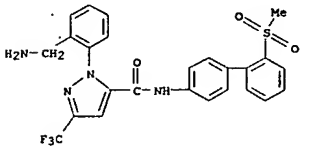
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



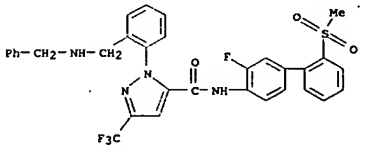
RN 228257-56-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)-4-methoxyphenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)



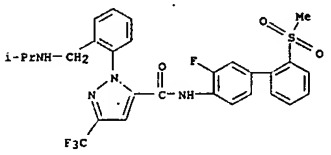
RN 228258-43-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)



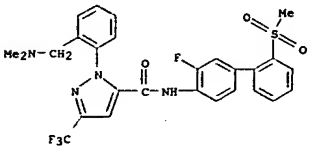
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 875139-46-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[2-[[(phenylmethyl)amino]methyl]phenyl]-3-(trifluoromethyl)-
(9CI)
(CA INDEX NAME)



RN 875139-51-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[2-[[(1-methylethyl)amino]methyl]phenyl]-3-(trifluoromethyl)-
(9CI) (CA INDEX NAME)

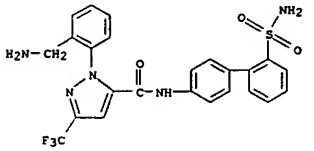


RN 875139-66-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-[(dimethylamino)methyl]phenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

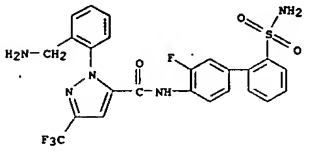


RN 875139-67-6 CAPLUS

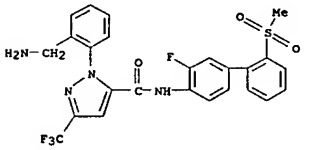
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 228258-44-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-
(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX
NAME)



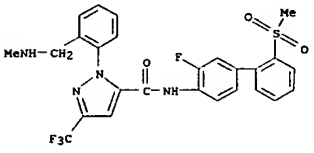
RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-
3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-46-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[3-fluoro-2'-
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)



L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR
THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L9 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1021642 CAPLUS
DOCUMENT NUMBER: 143:311996
TITLE: Methods for inhibiting platelet activation and aggregation, and therapeutic uses for conditions or surgical procedures that may result in unwanted platelet aggregation
INVENTOR(S): Porter, Stephen R.; Flaharty, Kristen K.; Tcheng, James E.; Ferkany, John W.
PATENT ASSIGNEE(S): Vddi Pharmaceuticals, USA
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005087266 | A1 | 20050922 | WO 2005-US7440 | 20050307 |

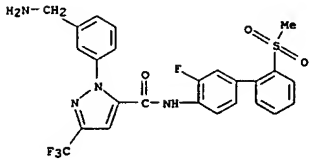
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-550792P P 20040305

AB The invention features methods for preventing platelet activation and aggregation and for treating individuals suffering from conditions or undergoing procedures that may result in unwanted platelet aggregation. The methods are based on the i.v., s.c., or transdermal administration of a platelet activation or aggregation inhibitor, e.g., xemilofiban, followed by oral administration of the same or a different platelet activation or aggregation inhibitor. The treatment may commence prior to a medical or surgical procedure or after the outbreak of an adverse medical condition, either of which results in the activation of platelets that may lead to thrombus formation, and may continue thereafter.

IT 292135-59-2, DPC423
RL: ANT (Analyte); ANST (Analytical study)
(combination therapy for inhibition of platelet aggregation)
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

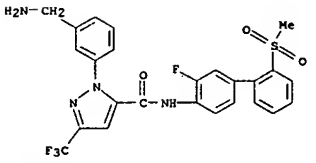
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L9 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:777848 CAPLUS
DOCUMENT NUMBER: 145:262418
TITLE: A Critical Assessment of Docking Programs and Scoring Functions
AUTHOR(S): Warren, Gregory L.; Andrews, C. Webster; Capelli, Anna-Maria; Clarke, Brian; LaLonde, Judith; Lambert, Millard H.; Lindvall, Mika; Nevins, Neysa; Semus, Simon F.; Senger, Stefan; Tedesco, Giovanna; Wall, Ian D.; Woolven, James M.; Peishoff, Catherine E.; Head, Martha S.
CORPORATE SOURCE: GlaxoSmithKline Pharmaceuticals, Collegeville, PA, 19426, USA
SOURCE: Journal of Medicinal Chemistry (2006), 49(20), 5912-5931
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Docking is a computational technique that samples conformations of small mols. in protein binding sites; scoring functions are used to assess which of these conformations best complements the protein binding site. An evaluation of 10 docking programs and 37 scoring functions was conducted against eight proteins of seven protein types for three tasks: binding mode prediction, virtual screening for lead identification, and rank-ordering by affinity for lead optimization. All of the docking programs were able to generate ligand conformations similar to crystallog. determined protein/ligand complex structures for at least one of the targets. However, scoring functions were less successful at distinguishing the crystallog. conformation from the set of docked poses. Docking programs identified active compds. from a pharmaceutically relevant pool of decoy compds.; however, no single program performed well for all of the targets. For prediction of compound affinity, none of the docking programs or scoring functions made a useful prediction of ligand binding affinity.

IT 209957-47-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(critical assessment of docking programs and scoring functions)
RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

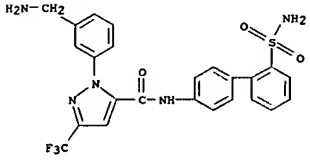
L9 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:511199 CAPLUS
DOCUMENT NUMBER: 143:145801
TITLE: Ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling
AUTHOR(S): Taha, Mutasem O.; Qandil, Amjad M.; Zaki, Dhia D.; AlDamen, Murad A.
CORPORATE SOURCE: Faculty of Pharmacy, Department of Pharmaceutical Sciences, University of Jordan, Amman, Jordan
SOURCE: European Journal of Medicinal Chemistry (2005), 40(7), 701-727
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The flexibility of activated factor X (fXa) binding site was assessed employing ligand-based pharmacophore modeling combined with genetic algorithm (GA)-based QSAR modeling. Four training subsets of wide structural diversity were selected from a total of 199 direct fXa inhibitors and were employed to generate different fXa pharmacophoric hypotheses using CATALYST software over two subsequent stages. In the first stage, high quality binding models (hypotheses) were identified. However, in the second stage, these models were refined by applying variable feature weight anal. to assess the relative significance of their features in the ligand-target affinity. The binding models were validated according to their coverage (capacity as a three-dimensional (3D) database search queries) and predictive potential as three-dimensional quant. structure-activity relationship (3D-QSAR) models. Subsequently, GA and multiple linear regression (MLR) anal. were employed to construct different QSAR models from high quality pharmacophores and explore the statistical significance of combination models in explaining bioactivity variations across 199 fXa inhibitors. Three orthogonal pharmacophoric models emerged in the optimal QSAR equation suggesting they represent three binding modes accessible to ligands in the binding pocket within fXa.

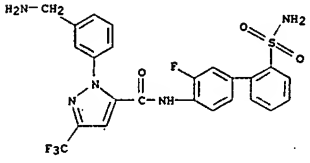
IT 209954-59-6 209955-48-6 209955-60-2 209957-35-7 209957-47-1 209957-51-7 209957-53-9
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling)

RN 209954-59-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

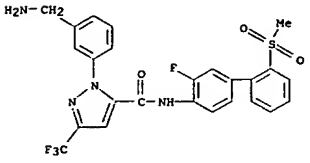
L9 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

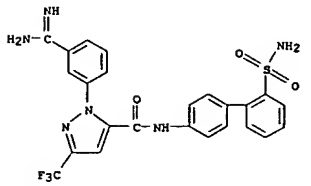


RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

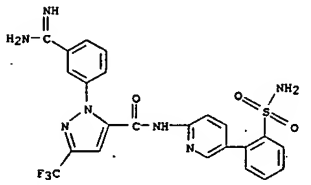


RN 209957-51-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

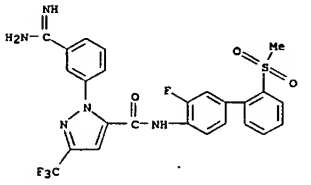


RN 209955-48-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

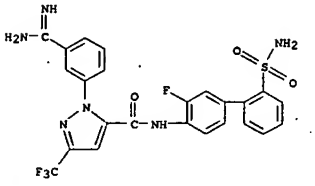


RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-53-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



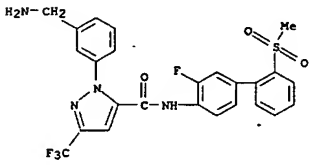
REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 10 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1151496 CAPLUS
DOCUMENT NUMBER: 142:328858
TITLE: The chimpanzee (Pan troglodytes) as a pharmacokinetic model for selection of drug candidates: Model characterization and application
AUTHOR(S): Wong, Harvey; Grossman, Scott J.; Bai, Stephen A.; Diamond, Sharon; Wright, Matthew R.; Grace, James E., Jr.; Qian, Mingxin; He, Kan; Yeleswaram, Krishnaswamy; Christ, David D.
CORPORATE SOURCE: Metabolism and Pharmacokinetics, Bristol-Myers Squibb Company, Wallingford, CT, USA
SOURCE: Drug Metabolism and Disposition (2004), 32(12), 1359-1369
CODEN: DMDSAI; ISSN: 0090-9556
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The chimpanzee (CHP) was evaluated as a pharmacokinetic model for humans (HUMs) using propranolol, verapamil, theophylline, and 12 proprietary compds. Species differences were observed in the systemic clearance of theophylline (.apprx.5-fold higher in CHPs), a low clearance compound, and the bioavailability of propranolol and verapamil (lower in CHPs), both high clearance compds. The systemic clearance of propranolol (.apprx.1.53 l/h/kg) suggested that the hepatic blood flow in CHPs is comparable to that in humans. No substantial differences were observed in the in vitro protein binding. A preliminary attempt was made to characterize cytochrome P 450 activities in CHP and HUM liver microsomes. Testosterone 6β-hydroxylation and tolbutamide methylhydroxylation activities were comparable in CHP and HUM liver microsomes. In contrast, dextromethorphan O-demethylation and phenacetin O-deethylation activities were .apprx.10-fold higher (per mg protein) in CHP liver microsomes. Intrinsic clearance ests. in CHP liver microsomes were higher for propranolol (.apprx.10-fold) and theophylline (.apprx.5-fold) and similar for verapamil. Of the 12 proprietary compds., 3 had oral clearances that differed in the two species by more than 3-fold, an acceptable range for biol. variability. Most of the observed differences are consistent with species differences in P 450 enzyme activity. Oral clearances of proprietary compds. in HUMs were significantly correlated to those from CHPs ($r = 0.68$; $p = 0.015$), but not to ests. from rat, dog, and monkey. In summary, the chimpanzee serves as a valuable surrogate model for human pharmacokinetics, especially when species differences in P 450 enzyme activity are considered.

IT 292135-59-2, DPC 423
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(chimpanzee (Pan troglodytes) as a surrogate model for human pharmacokinetic studies in relation to species differences in P 450 enzyme activity)

L9 ANSWER 10 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:799558 CAPLUS
DOCUMENT NUMBER: 141:296012
TITLE: Preparation of factor Xa- and thrombin-inhibiting substituted benzamidines and sulfonylbenzamidines as potential anticoagulants
INVENTOR(S): Pinto, Donald J.; Qiao, Jennifer X.; Gangor, Timur; Lam, Patrick Y. S.; Li, Yun-long
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 279 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004083174 | A2 | 20040930 | WO 2004-US8033 | 20040317 |
| WO 2004083174 | A3 | 20041125 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2004209863 | A1 | 20041021 | US 2004-801518 | 20040316 |
| US 7122557 | B2 | 20061017 | | |
| EP 1603562 | A2 | 20051214 | EP 2004-757516 | 20040317 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK | | | | |

PRIORITY APPLN. INFO.: US 2003-455709P P 20030318
US 2004-801518 A 20040316
WO 2004-US8033 W 20040317

OTHER SOURCE(S): MARPAT 141:296012
GI

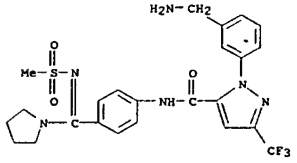
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. P4-M-M4 (I) [M = (un)substituted 3-10 membered carbocyclic or a 4-10 membered heterocyclic ring containing 1-3 O, N, or S atoms, alone or fused to an (un)substituted 5-7 membered carbocycle or heterocycle; P4 = Z-A-B; M4 = G-G1; A = (un)substituted 3-10 membered carbocyclic or 5-12 membered heterocyclic ring ; B = (un)substituted amidino, guanidino, iminomethyl; G = five or six-membered carbocycle or heterocycle fused to a benzene, pyridine, pyrimidine, pyrazine, or pyridazine ring; G1 = bond, (un)substituted alkyl, alkenyl, alkynyl; Z = (un)substituted alkylene], such as tetrahydropyrazolo[3,4-c]pyridinone II or

L9 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(pyridinylaminocarbonylphenylaminocarbonyl)benzamidine III are prepd. as inhibitors of Factor Xa and thrombin for use as anticoagulants. Deprotonation of 2-amino-4-chloropyridine and addn. to 5-chloroisatoic anhydride yields N-(5-chloro-2-pyridinyl) 2-amino-5-chlorobenzamide (IV). Acid-mediated addn. of dimethylamine to the nitrile of Me 4-cyanobenzoate, mesylation of the amidine nitrogen, and base-mediated hydrolysis of the ester yields 4-(N,N-dimethyl-N'-methylsulfonylamidino)benzoic acid (V). Coupling of IV and V mediated by BOP yields III. Some compds. of the invention inhibit human factor Xa with Ki values of ≤ 10 μM; in addn., some of the invention compds. inhibit thrombin in vitro..(no data).

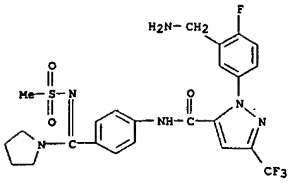
IT 764658-97-1P 764658-98-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of factor Xa- and thrombin-inhibiting substituted benzamidines and sulfonylbenzamidines as potential anticoagulants)

RN 764658-97-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[[(methylsulfonyl)imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)



RN 764658-98-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[4-[[(methylsulfonyl)imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

L9 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:791919 CAPLUS
DOCUMENT NUMBER: 141:342889
TITLE: SAR and factor IXa crystal structure of a dual inhibitor of factors IXa and Xa
AUTHOR(S): Smallheer, Joanne M.; Alexander, Richard S.; Wang, Jianmin; Wang, Shuaige; Nakajima, Suanne; Rossi, Karen A.; Smallwood, Angela; Barbera, Frank; Burdick, Debra; Luettgen, Joseph M.; Knabb, Robert M.; Wexler, Ruth R.; Jadhav, Prabhakar K.
CORPORATE SOURCE: Bristol-Myers Squibb Company, Princeton, NJ, 08543-5400, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(21), 5263-5267
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:342889

AB Modifications to the P4 moiety and pyrazole C3 substituent of factor Xa inhibitor SN-429 provided several new compds., which are 5-10 nM inhibitors of factor IXa. An x-ray crystal structure of one example complexed to factor IXa shows that these compds. adopt a similar binding mode to that previously observed with pyrazole inhibitors in the factor Xa active site both with regard to how the inhibitor binds and the position of Tyr99.

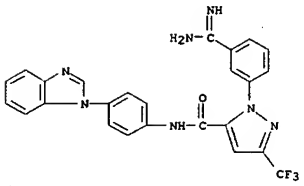
IT 848393-61-3P 848393-63-5P 848393-64-6P
848393-85-1P 848393-86-2P 848393-88-4P
848393-89-5P 848393-91-9P 848393-92-0P
848393-93-1P 848393-95-3P 848393-96-4P
848393-97-5P 848393-98-6P 848393-99-7P
848394-00-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(pyrazole compds. preparation, crystal structure, and dual inhibition of factors IXa and Xa)

RN 848393-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-45-0
CMF C25 H18 F3 N7 O

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



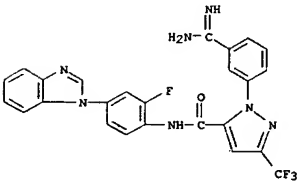
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 848393-63-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-46-1
CMF C25 H17 F4 N7 O



CM 2

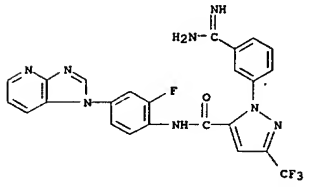
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 76-05-1
CMF C2 H F3 O2

RN 848393-64-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-imidazo[4,5-b]pyridin-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-47-2
CMF C24 H16 F4 N8 O



CM 2

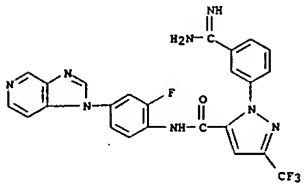
CRN 76-05-1
CMF C2 H F3 O2

RN 848393-85-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-imidazo[4,5-c]pyridin-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-48-3

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C24 H16 F4 N8 O



CM 2

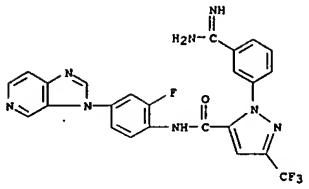
CRN 76-05-1
CMF C2 H F3 O2

RN 848393-86-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(3H-imidazo[4,5-c]pyridin-3-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-49-4
CMF C24 H16 F4 N8 O

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



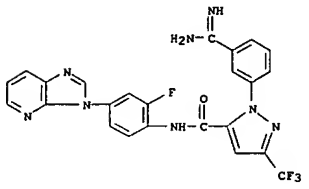
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 848393-88-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(3H-imidazo[4,5-b]pyridin-3-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-50-7
CMF C24 H16 F4 N8 O



L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

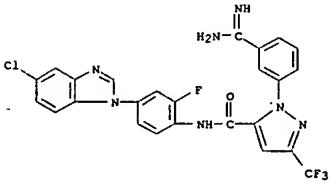
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 848393-89-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-chloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-51-8
CMF C25 H16 Cl F4 N7 O



CM 2

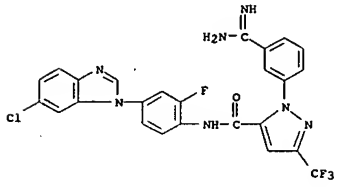
CRN 76-05-1
CMF C2 H F3 O2

RN 848393-91-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(6-chloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 774218-52-9
CMF C25 H16 Cl F4 N7 O



CM 2

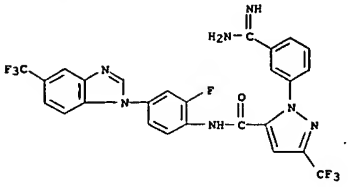
CRN 76-05-1
CMF C2 H F3 O2

RN 848393-92-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-[5-(trifluoromethyl)-1H-benzimidazol-1-yl]phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-53-0
CMF C26 H16 F7 N7 O

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

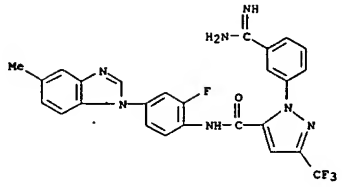
CRN 76-05-1
CMF C2 H F3 O2

RN 848393-93-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-methyl-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-54-1
CMF C26 H19 F4 N7 O

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



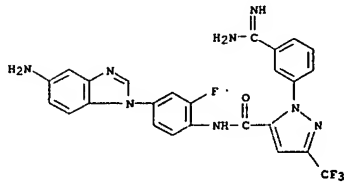
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 848393-95-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-(5-amino-1H-benzimidazol-1-yl)-2-fluorophenyl]-1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-55-2
CMF C25 H18 F4 N8 O



L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

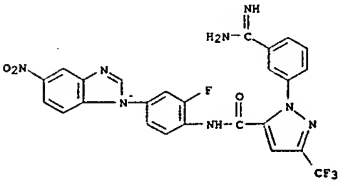
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 848393-96-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-nitro-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-56-3
CMF C25 H16 F4 N8 O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

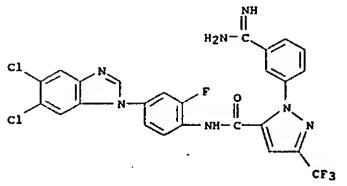
RN 848393-97-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5,6-dichloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-,

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-57-4
CMF C25 H15 Cl2 F4 N7 O



CM 2

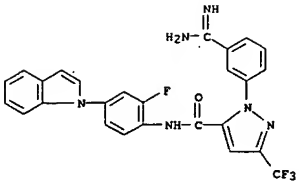
CRN 76-05-1
CMF C2 H F3 O2

RN 848393-98-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-indol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-58-5
CMF C26 H18 F4 N6 O

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



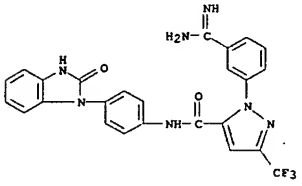
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 848393-99-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

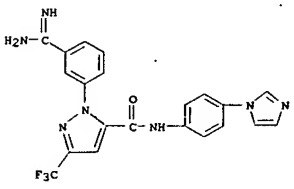
CRN 774218-59-6
CMF C25 H18 F3 N7 O2



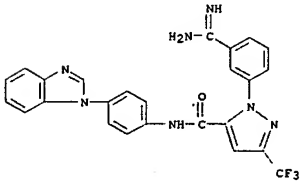
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 209956-75-2P 774218-45-0P 774218-46-1P
774218-47-2P 774218-48-3P 774218-49-4P
774218-50-7P 774218-51-8P 774218-52-9P
774218-53-0P 774218-54-1P 774218-55-2P
774218-56-3P 774218-57-4P 774218-58-5P
774218-59-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(pyrazole compds. preparation, crystal structure, and dual inhibition of
factors IXa and Xa)

RN 209956-75-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 774218-45-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 774218-46-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

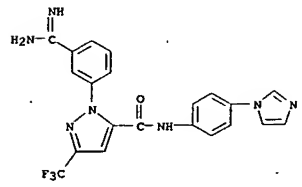
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 848394-00-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

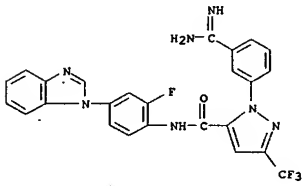
CRN 209956-75-2
CMF C21 H16 F3 N7 O



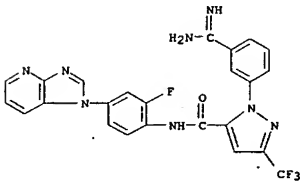
CM 2

CRN 76-05-1
CMF C2 H F3 O2

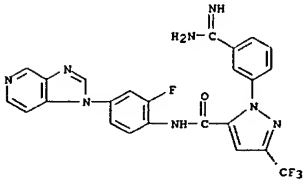
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 774218-47-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-imidazo[4,5-b]pyridin-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

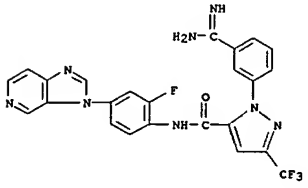


RN 774218-48-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-imidazo[4,5-c]pyridin-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

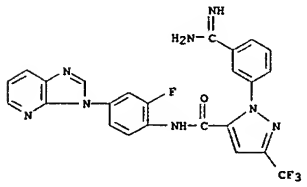


RN 774218-49-4 CAPLUS

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(3H-imidazo[4,5-c]pyridin-3-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

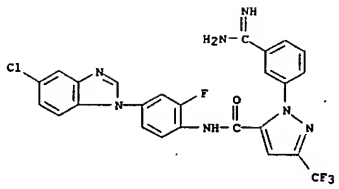


RN 774218-50-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(3H-imidazo[4,5-b]pyridin-3-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

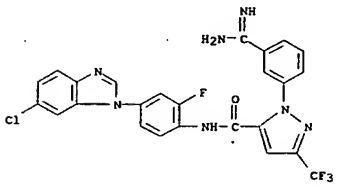


RN 774218-51-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-chloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

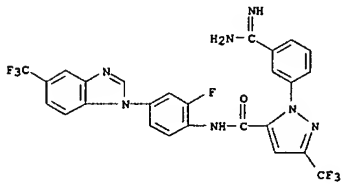


RN 774218-52-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(6-chloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

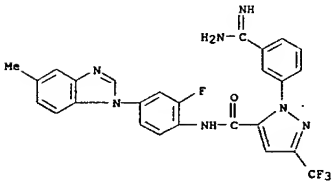


RN 774218-53-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-[5-(trifluoromethyl)-1H-benzimidazol-1-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

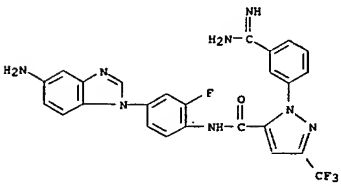
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



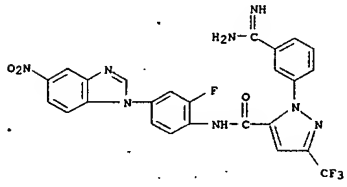
RN 774218-54-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-methyl-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



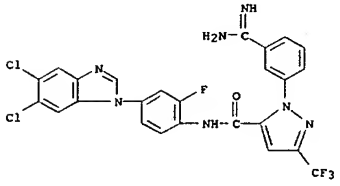
RN 774218-55-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-(5-amino-1H-benzimidazol-1-yl)-2-fluorophenyl]-1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 774218-56-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-nitro-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

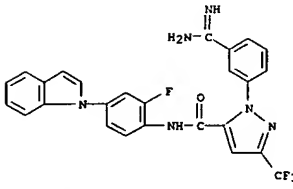


RN 774218-57-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5,6-dichloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

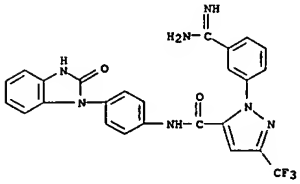


RN 774218-58-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-indol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 774218-59-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

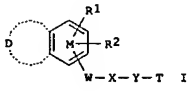
ACCESSION NUMBER: 2004:20490 CAPLUS
DOCUMENT NUMBER: 140:77148
TITLE: Preparation of N-[4-(thiooxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis
INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsaklakidis, Christos; Gleitz, Johannes; Barnes, Christopher
PATENT ASSIGNEE(S): Merck Patent Gmbh, Germany
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004002477 | A1 | 20040108 | WO 2003-EP5898 | 20030605 |
| WO 2004002477 | A8 | 20040415 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| DE 10229070 | A1 | 20040115 | DE 2002-10229070 | 20020628 |
| CA 2491271 | A1 | 20040108 | CA 2003-2491271 | 20030605 |
| AU 2003238475 | A1 | 20040119 | AU 2003-238475 | 20030605 |
| EP 1517685 | A1 | 20050330 | EP 2003-732540 | 20030605 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| JP 2005535630 | T | 20051124 | JP 2004-516575 | 20030605 |
| EP 1679073 | A1 | 20060712 | EP 2006-157 | 20030605 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, SK | | | | |
| US 2005203127 | A1 | 20050915 | US 2004-519356 | 20041228 |

PRIORITY APPLN. INFO.: DE 2002-10229070 A 20020628
EP 2003-732540 A3 20030605
WO 2003-EP5898 W 20030605

OTHER SOURCE(S): MARPAT 140:77148
GI

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



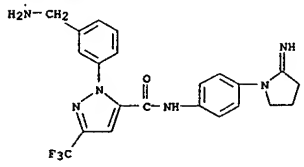
AB Title compds. [I; D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene; M = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(:S)N(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bi)cyclic aromatic (hetero)cyclyl; X = CONR3, CONR3C(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y = alkylene, cycloalkylene, heterodiyl, aryldiyl; T = (substituted) (bi)cyclic aromatic heterocyclyl], were prepared Thus, 333 mg

{3-[5-(4-[2-iminopyrrolidin-1-yl]phenylcarbamoyl)-3-trifluoromethylpyrazol-1-yl]benzyl}carbamic acid tert-Bu ester (preparation given) in EtOH was treated with HCl in ether to give 289 mg N-[4-(2-iminopyrrolidin-1-yl)phenyl]-1-(3-aminomethylphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the receptor Xa with IC50 = 9,6·10-9 M and to the receptor VIIa with IC50 = 2,3·10-8 M.

IT 640287-97-4P 640288-03-5P 640288-05-7P
640288-06-8P 640288-07-9P 640288-11-5P
640288-12-6P 640288-13-7P 640288-20-6P
640288-21-7P 640288-22-8P 640288-23-9P
640288-24-0P 640288-25-1P 640288-26-2P
640288-27-3P 640288-28-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

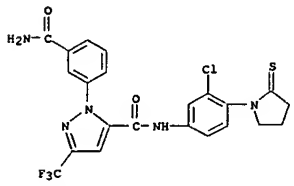
RN 640287-97-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

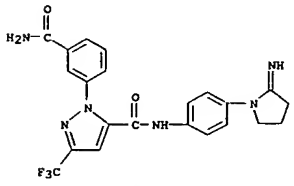


●2 HCl

RN 640288-03-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-chloro-4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

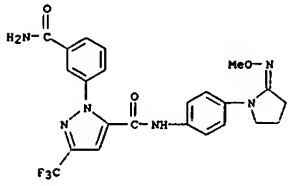


RN 640288-05-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

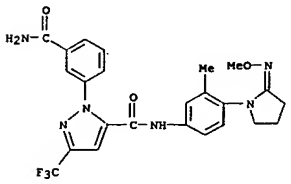


RN 640288-06-8 CAPLUS

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

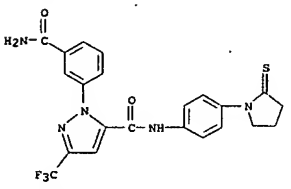


RN 640288-07-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]-3-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

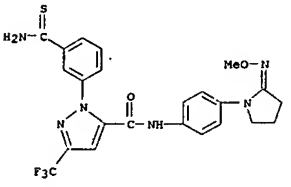


RN 640288-11-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-bromo-4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

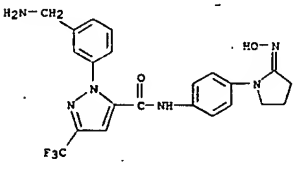
L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 640288-20-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminothioxomethyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

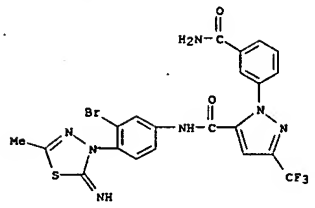


RN 640288-21-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[2-(hydroxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

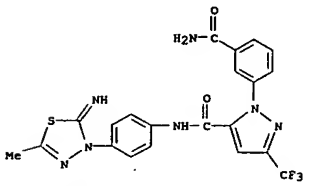


RN 640288-22-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-amino-4,5-dihydro-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

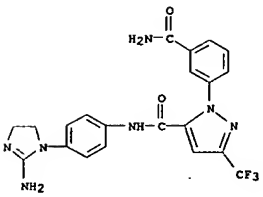


RN 640288-12-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

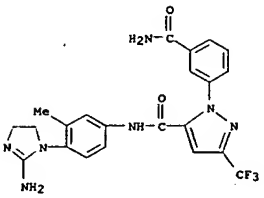


RN 640288-13-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
NAME)

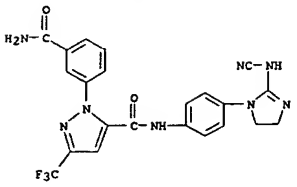


RN 640288-23-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-amino-4,5-dihydro-1H-imidazol-1-yl)-3-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

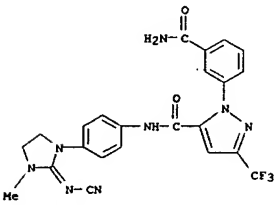


RN 640288-24-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(cyanoamino)-4,5-dihydro-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

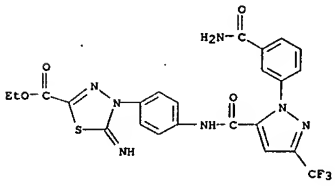


RN 640288-25-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(cyanoimino)-3-methyl-1-imidazolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

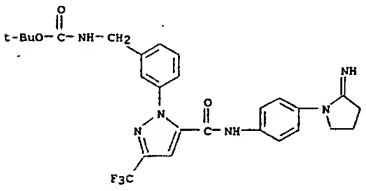


RN 640288-26-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(5-ethyl-2-imino-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

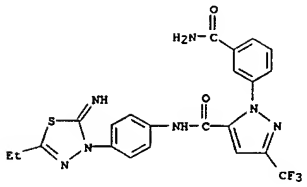


IT 640288-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)
RN 640288-00-2 CAPLUS
CN Carbamic acid, [[3-[5-[[[4-(2-imino-1-pyrrolidinyl)phenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

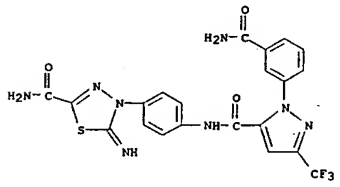


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 640288-27-3 CAPLUS
CN 1,3,4-Thiadiazole-2-carboxamide, 4-[4-[[[1-[3-(aminocarbonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-4,5-dihydro-5-imino- (9CI) (CA INDEX NAME)



RN 640288-28-4 CAPLUS
CN 1,3,4-Thiadiazole-2-carboxylic acid, 4-[4-[[[1-[3-(aminocarbonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-4,5-dihydro-5-imino-, ethyl ester (9CI) (CA INDEX NAME)

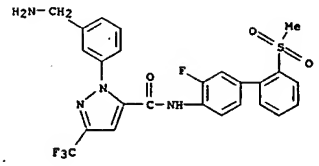
L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:844982 CAPLUS
DOCUMENT NUMBER: 140:59557
TITLE: Discovery of 1-(2-Aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl)]-4-yl]-1H-pyrazole-5-carboxamide (DPC602), a Potent, Selective, and Orally Bioavailable Factor Xa Inhibitor
AUTHOR(S): Pruitt, James R.; Pinto, Donald J. P.; Galemmo, Robert A., Jr.; Alexander, Richard S.; Rossi, Karen A.; Wells, Brian L.; Drummond, Spencer; Bostrom, Lori L.; Burdick, Debra; Bruckner, Robert; Chen, Haiying; Smallwood, Angela; Wong, Pancras C.; Wright, Matthew R.; Bai, Steven; Luettgen, Joseph M.; Knabb, Robert M.; Lam, Patrick Y. S.; Wexler, Ruth R.
CORPORATE SOURCE: Pharmaceutical Research Institute, Bristol-Myers Squibb Company, Pennington, NJ, 08534, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(25), 5298-5315
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:59557

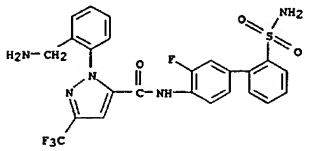
AB Factor Xa, a serine protease, is at the critical juncture between the intrinsic and extrinsic pathways of the coagulation cascade. Inhibition of factor Xa has the potential to provide effective treatment for both venous and arterial thrombosis. The authors recently described a series of meta-substituted phenylpyrazoles that are highly potent, selective, and orally bioavailable factor Xa inhibitors. In this paper, the authors report their efforts to further optimize the selectivity profile of the factor Xa inhibitors with a series of ortho- and/or para-substituted phenylpyrazole derivs. The most potent compds. display sub-nanomolar inhibition consts. for factor Xa and show greater than 1000-fold selectivity against other serine proteases. These compds. are also effective in a rabbit model of arteriovenous shunt thrombosis. Optimization of this series led to the preclin. development of DPC602, a 2-(aminomethyl)phenylpyrazole analog, as a highly potent, selective, and orally bioavailable factor Xa inhibitor.

IT 209957-47-1DP, factor Xa complex 228258-45-5DP, factor Xa complex
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure of)
RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-
3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

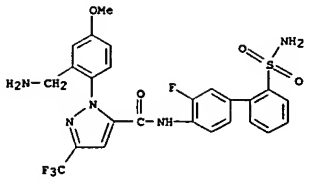


IT 228258-59-1P 228258-62-6P 228258-85-3P
228258-86-4P 228258-87-5P 637318-67-3P
637318-69-5P 637318-85-5P 637319-02-9P
637319-13-2P 637319-15-4P 637319-17-6P
637319-19-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of
1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl]]-4-yl]-1H-pyrazole-5-carboxamide and related compds. as orally bioavailable factor Xa inhibitors)
RN 228258-59-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-50-9
CMF C25 H21 F4 N5 O4 S

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



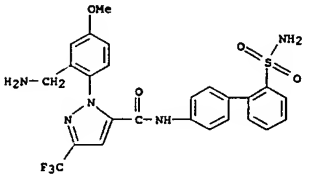
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-62-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-38-3
CMF C25 H22 F3 N5 O4 S



L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

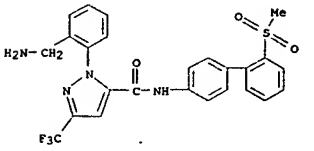
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-85-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-43-3
CMF C25 H21 F3 N4 O3 S



CM 2

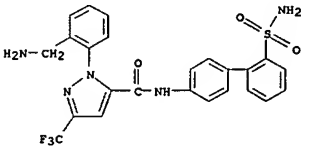
CRN 76-05-1
CMF C2 H F3 O2

RN 228258-86-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-44-4
CMF C24 H20 F3 N5 O3 S

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



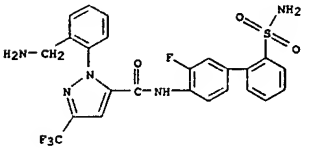
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-87-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-
3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
mono(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM 1

CRN 228258-45-5
CMF C24 H19 F4 N5 O3 S



CM 2

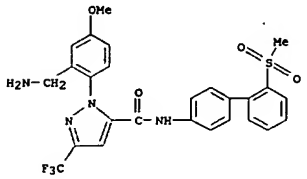
CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 637318-67-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, trifluoroacetate (10:13) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-44-1
CMF C26 H23 F3 N4 O4 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 637318-69-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, trifluoroacetate (2:3) (9CI) (CA INDEX NAME)

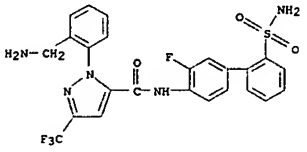
CM 1

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 637319-02-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

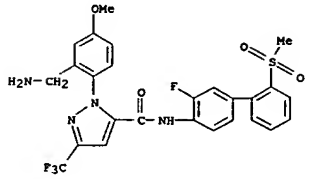
RN 637319-13-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 875139-67-6
CMF C26 H22 F4 N4 O3 S

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 228257-56-5
CMF C26 H22 F4 N4 O4 S



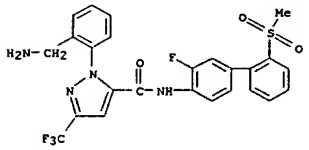
CM 2

CRN 76-05-1
CMF C2 H F3 O2

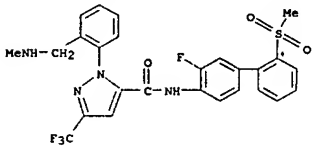
RN 637318-85-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, trifluoroacetate (10:11) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-46-6
CMF C25 H20 F4 N4 O3 S



L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



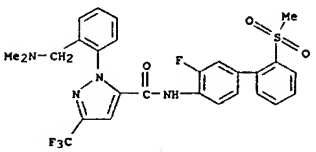
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 637319-15-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[(dimethylamino)methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 875139-66-5
CMF C27 H24 F4 N4 O3 S



CM 2

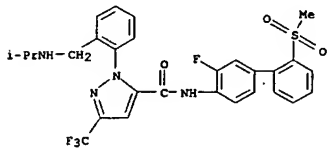
CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 637319-17-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[2-[[(1-methylethyl)amino]methyl]phenyl]-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 875139-51-8
CMF C28 H26 F4 N4 O3 S



CM 2

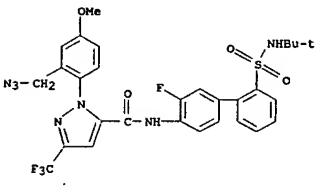
CRN 76-05-1
CMF C2 H F3 O2

RN 637319-19-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[2-[[(phenylmethyl)amino]methyl]phenyl]-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

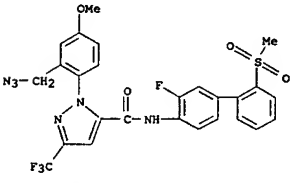
CM 1

CRN 875139-46-1

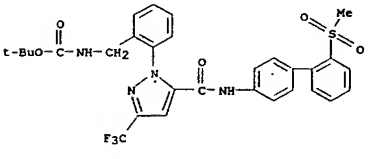
L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228259-22-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(azidomethyl)-4-methoxyphenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

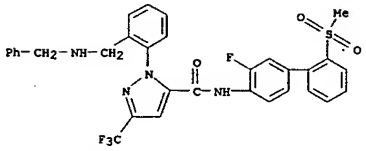


RN 228259-36-7 CAPLUS
CN Carbamic acid, [[2-[5-[[[2'-(methylsulfonyl)[1,1'-biphenyl]-4-
yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 228259-37-8 CAPLUS
CN Carbamic acid, [[2-[5-[[[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-
biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-
yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C32 H26 F4 N4 O3 S

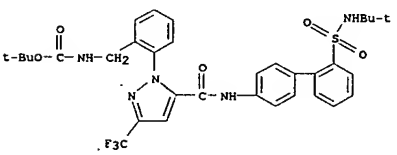


CM 2

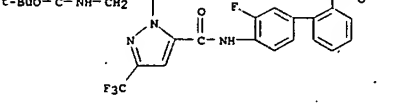
CRN 76-05-1
CMF C2 H F3 O2

IT 228259-20-9P 228259-22-1P 228259-36-7P
228259-37-8P 228259-38-9P 228259-39-0P
637319-00-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of
1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-
(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1H-pyrazole-5-carboxamide and
related compds. as orally bioavailable factor Xa inhibitors)
RN 228259-20-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[2'-
[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-
(trifluoromethyl)- (9CI) (CA INDEX NAME)

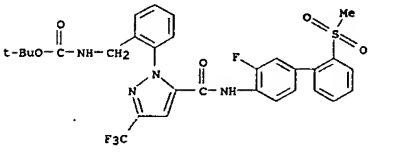
L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228259-38-9 CAPLUS
CN Carbamic acid, [[2-[5-[[[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-
fluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-
1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

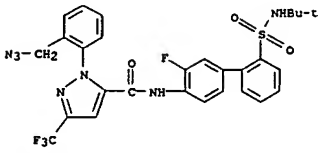


RN 228259-39-0 CAPLUS
CN Carbamic acid, [[2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-
yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 637319-00-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)phenyl]-N-[2'-[[(1,1-
dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-
(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT .

L9 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

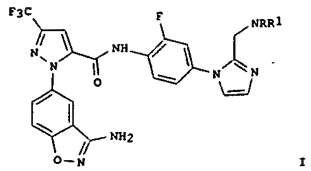
ACCESSION NUMBER: 2003:454067 CAPLUS
DOCUMENT NUMBER: 139:36524
TITLE: Preparation of novel N-[4-(1H-imidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamides as factor Xa inhibitors
INVENTOR(S): Quan, Mimi L.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003047517 | A2 | 20030612 | WO 2002-US38168 | 20021126 |
| WO 2003047517 | A3 | 20040226 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2003144287 | A1 | 20030731 | US 2002-302184 | 20021122 |
| US 6730689 | B2 | 20040504 | | |
| AU 2002352962 | A1 | 20030617 | AU 2002-352962 | 20021126 |
| EP 1460996 | A2 | 20040929 | EP 2002-789922 | 20021126 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| HU 200402515 | A2 | 20050329 | HU 2004-2515 | 20021126 |
| JP 2005527485 | T | 20050915 | JP 2003-548778 | 20021126 |

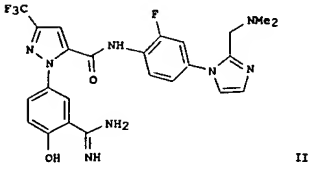
PRIORITY APPLN. INFO.: US 2001-336972P P 20011204
WO 2002-US38168 W 20021126

OTHER SOURCE(S): MARPAT 139:36524
GI

L9 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I



II

AB N-[4-(1H-imidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamides of formula I [R = H, alkyl; R1 = H, acyl, etc.] and derivs. thereof are prepared which are useful as inhibitors of factor Xa. Thus, II was prepared in several steps. The prepared compds. had Ki values of ≤ 10 μM against human factor Xa.

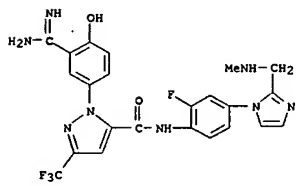
IT 540510-36-9P 540510-43-8P
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazolylphenyl pyrazolecarboxamide derivs. as factor Xa inhibitors)

RN 540510-36-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)-4-hydroxyphenyl]-N-[2-fluoro-4-[2-[(methylamino)methyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 540510-35-8
CMF C23 H20 F4 N8 O2

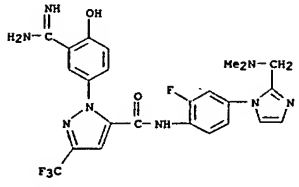
L9 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 540510-43-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)-4-hydroxyphenyl]-N-[4-[2-[(dimethylamino)methyl]-1H-imidazol-1-yl]-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

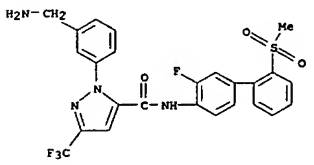


L9 ANSWER 16 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:363518 CAPLUS
DOCUMENT NUMBER: 140:16
TITLE: Factor Xa inhibitors: Today and beyond
AUTHOR(S): Walenga, Jeanine M.; Jeske, Walter P.; Hoppensteadt, Debra; Fareed, Jawed
CORPORATE SOURCE: Department of Pathology, Loyola University Medical Center, Maywood, IL, 60153, USA
SOURCE: Current Opinion in Investigational Drugs (Thomson Current Drugs) (2003), 4(3), 272-281
CODEN: COIDAZ; ISSN: 1472-4472
PUBLISHER: Thomson Current Drugs
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review. Serine proteases play an important role in thrombogenesis, the process that leads to blood clotting and conditions such as heart attack, stroke and other cardiovascular disorders. In the coagulation network, the activation of various serine proteases facilitates the formation of the serine protease Factor Xa, which plays a central role in the process of coagulation and platelet activation. Factor Xa is an essential component of the prothrombinase complex, from which thrombin is formed, which then directly leads to fibrin clot formation. Thus, the inhibition of Factor Xa and its generation is an important strategy in the development of new antithrombotic drugs.

IT 292135-59-2, DPC-423
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(factor Xa inhibitors as antithrombotic drugs)

RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

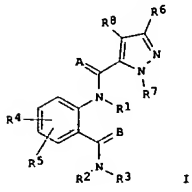
REFERENCE COUNT: 120 THERE ARE 120 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:242097 CAPLUS
DOCUMENT NUMBER: 138:267201
TITLE: Pesticidal compositions for coating plant propagation material containing anthranilamides
INVENTOR(S): Berger, Richard Alan; Flexner, John Lindsey
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 147 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003024222 | A1 | 20030327 | WO 2002-US30302 | 20020910 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2458163 | A1 | 20030327 | CA 2002-2458163 | 20020910 |
| EP 1427285 | A1 | 20040616 | EP 2002-775972 | 20020910 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| BR 2002012993 | A | 20040817 | BR 2002-12993 | 20020910 |
| JP 2005502716 | T | 20050127 | JP 2003-528126 | 20020910 |
| JP 3770495 | B2 | 20060426 | | |
| HU 200401893 | A2 | 20050128 | HU 2004-1893 | 20020910 |
| NZ 532269 | A | 20051028 | NZ 2002-532269 | 20020910 |
| CN 1713819 | A | 20051228 | CN 2002-818578 | 20020910 |
| ZA 2004000413 | A | 20050120 | ZA 2004-413 | 20040120 |
| US 2004209923 | A1 | 20041021 | US 2004-485125 | 20040126 |
| PRIORITY APPLN. INFO.: | | | US 2001-323941P P | 20010921 |
| | | | WO 2002-US30302 W | 20020910 |

OTHER SOURCE(S): MARPAT 138:267201
GI

L9 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

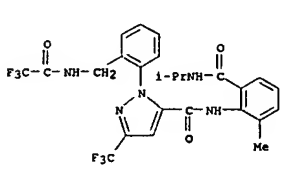


I

AB An invertebrate pest control composition for coating a propagule comprises (1)
a biol. effective amount of an anthranilamide compds. I (Markush included),
an N-oxide thereof or an agriculturally suitable salt thereof, and (2) a film former or adhesive agent. Arthropodicidal composition containing anthranilamide compds. I may further comprise addnl. biol. active compds. selected from arthropodicides of the group consisting of pyrethroids, carbamates, neonicotinoids, neuronal sodium channel blockers, insecticidal
macrocyclic lactones, γ-aminobutyric acid (GABA) antagonists, insecticidal ureas, and juvenile hormone mimics, and fungicides. The propagule is a seed of cotton, maize, soybean, rice, etc., or a rhizome, tuber, bulb or corm, or viable division thereof, of potato, sweet potato, garden onion, tulip, daffodil, crocus hyacinth, etc., or is a stem or leaf
cutting.

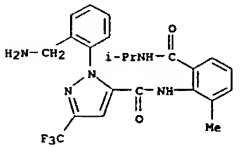
IT 500007-98-7 500007-99-8 500008-13-9
RL: AGR (Agricultural use); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(anthranilamide compds. as pesticides for plant propagation material)

RN 500007-98-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-methyl-6-[[(1-methylethyl)amino]carbonyl]phenyl]-1-[2-[[(trifluoroacetyl)amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



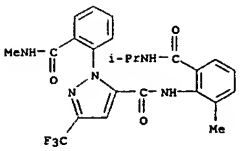
RN 500007-99-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-methyl-6-[[(1-

L9 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
methylethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 500008-13-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[(methylamino)carbonyl]phenyl]-N-[2-methyl-6-[[(1-methylethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



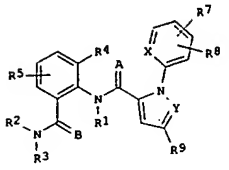
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:154408 CAPLUS
DOCUMENT NUMBER: 138:205054
TITLE: Preparation of substituted anthranilamides for controlling invertebrate pests
INVENTOR(S): Finkelstein, Bruce Lawrence; Lahm, George Philip; McCann, Stephen Frederick; Song, Ying; Stevenson, Thomas Martin
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003016284 | A1 | 20030227 | WO 2002-US26960 | 20020813 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1417176 | A1 | 20040512 | EP 2002-761486 | 20020813 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| BR 2002012183 | A | 20040824 | BR 2002-12183 | 20020813 |
| JP 2005503384 | T | 20050203 | JP 2003-521210 | 20020813 |
| CN 1653051 | A | 20050810 | CN 2002-816050 | 20020813 |
| US 2005282868 | A1 | 20051222 | US 2004-486312 | 20040722 |
| PRIORITY APPLN. INFO.: | | | US 2001-312680P | P 20010816 |
| | | | WO 2002-US26960 | W 20020813 |

OTHER SOURCE(S): MARPAT 138:205054
GI

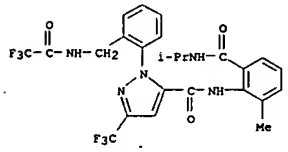
L9 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



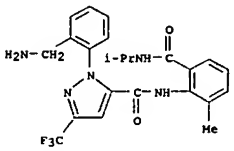
I

AB The title compds. [I; A, B = O, S; X = N, CR10; Y = N, CH; R1 = H, alkyl, cycloalkyl, etc.; R2 = alkyl, alkenyl, cycloalkyl, etc.; R3 = H, alkyl, alkenyl, etc.; NR2R3 = (un)substituted ring optionally containing addnl. heteroatom; R4 = alkyl, haloalkyl, CN, etc.; R5, R8 = H, alkyl, haloalkyl, etc.; R7 = H, alkyl, haloalkyl, etc.; R9 = CF3, OCF3, OCHF2, etc.; R10 = H, alkyl, haloalkyl, etc.], useful for controlling an invertebrate pest, were prepared E.g., a 3-step synthesis of I [A, B = O; X = CH; Y = N; R1 = H; R2 = iso-Pr; R3 = H; R4 = Me; R5 = H; R7 = 2-(CH2OH); R8 = H; R9 = CF3], starting from 1-[2-(methoxycarbonyl)phenyl]-3-trifluoromethyl-1H-pyrazole-5-carboxylic acid and 2-amino-3-methylbenzoic acid, which provided excellent levels of plant protection (20% or less damage) in biol. tests, was given.
IT 500007-98-7P 500028-35-3P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of substituted anthranilamides for controlling invertebrate pests)
RN 500007-98-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-methyl-6-[[(1-methylethyl)amino]carbonyl]phenyl]-1-[2-[[(trifluoroacetyl)amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 500028-35-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-methyl-6-[[(1-methylethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



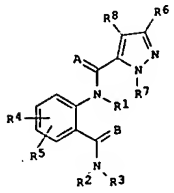
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:154154 CAPLUS
DOCUMENT NUMBER: 138:200331
TITLE: Method for controlling particular insect pests by applying anthranilamide compounds
INVENTOR(S): Lahm, George Philip; McCann, Stephen Frederick; Patel, Kanu Maganbhai; Selby, Thomas Paul; Stevenson, Thomas Martin
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 150 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003015518 | A1 | 20030227 | WO 2002-US25613 | 20020813 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2454302 | A1 | 20030227 | CA 2002-2454302 | 20020813 |
| EP 1416796 | A1 | 20040512 | EP 2002-752809 | 20020813 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| HU 200401043 | A2 | 20040928 | HU 2004-1043 | 20020813 |
| BR 2002012187 | A | 20041005 | BR 2002-12187 | 20020813 |
| CN 1541063 | A | 20041027 | CN 2002-815930 | 20020813 |
| JP 2004538327 | T | 20041224 | JP 2003-520289 | 20020813 |
| JP 3689817 | B2 | 20050831 | | |
| ZA 2004000033 | A | 20050803 | ZA 2004-33 | 20020813 |
| ZA 2004000034 | A | 20050803 | ZA 2004-34 | 20020813 |
| RU 2262231 | C1 | 20051020 | RU 2004-107513 | 20020813 |
| NZ 530442 | A | 20060728 | NZ 2002-530442 | 20020813 |
| ZA 2003009911 | A | 20050311 | ZA 2003-9911 | 20031222 |
| US 2005075372 | A1 | 20050407 | US 2004-483115 | 20040107 |
| JP 2005041880 | A | 20050217 | JP 2004-258923 | 20040906 |
| PRIORITY APPLN. INFO.: | | | US 2001-311919P | P 20010813 |
| | | | US 2001-324173P | P 20010921 |
| | | | US 2001-324128P | P 20010921 |
| | | | US 2002-369661P | P 20020402 |
| | | | JP 2003-520290 | A3 20020813 |
| | | | WO 2002-US25613 | W 20020813 |

OTHER SOURCE(S): MARPAT 138:200331
GI

L9 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



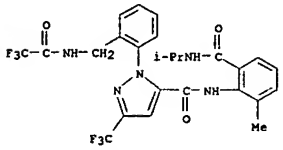
I

AB Anthranilamide compds. I (Markush included), N-oxides or an agriculturally
suitable salts thereof are prepared as insecticides for controlling lepidopteran, homopteran, hemipteran, thysanopteran and coleopteran insect
pests. Insecticidal composition containing anthranilamide compds. I may further
comprise addnl. biol. active compds. selected from arthropodicides of the group consisting of pyrethroids, carbamates, neonicotinoids, neuronal sodium channel blockers, insecticidal macrocyclic lactones, γ-aminobutyric acid (GABA) antagonists, insecticidal ureas, and juvenile hormone mimics.

IT 500007-98-7 500007-99-8 500008-13-9
RL: AGR (Agricultural use): BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(anthranilamide compds. as insecticides)

RN 500007-98-7 CAPLUS

CN 1H-Pyrazole-5-carboxamide, N-[2-methyl-6-[[(1-methylethyl)amino]carbonyl]phenyl]-1-[2-[[(trifluoroacetyl)amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

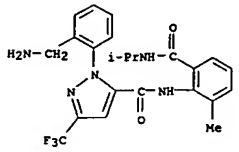


RN 500007-99-8 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-methyl-6-[[(1-

L9 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

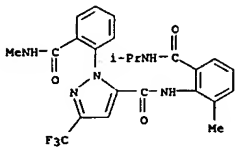
methylethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 500008-13-9 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[2-[(methylamino)carbonyl]phenyl]-N-[2-methyl-6-[[(1-methylethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 20 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:85815 CAPLUS
DOCUMENT NUMBER: 138:395309
TITLE: Development and validation of a liquid chromatography-mass spectrometric method for the determination of DPC 423, an antithrombotic agent, in rat and dog plasma
AUTHOR(S): Chi, Cecilia; Liang, Li; Padovani, Patty; Unger, Steve
CORPORATE SOURCE: Metabolism & Pharmacokinetics, PRI, Experimental Station, Bristol-Myers Squibb Company, Wilmington, DE, 19803-0353, USA
SOURCE: Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences (2003), 783(1), 163-172
CODEN: JCBAAI; ISSN: 1570-0232
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

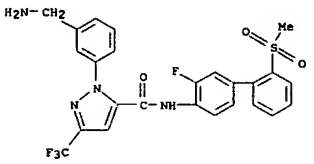
AB A sensitive and selective LC-MS-MS method for the determination of DPC 423 (I), an
antithrombotic agent, is described. This method used a solid-phase extraction
from 0.1 mL plasma with an Isolute C2 cartridge. HPLC separation was carried
out on a YMC ODS-AQ C18 column (50+2 mm) at a flow rate of 300 μL/min with an anal. time of 5 min. Compds. were eluted using a mobile phase of H2O/CH3CN/HCOOH:66:34:0.1 (volume/volume/volume), pH 4.0. A structural
analog of I was used as the internal standard to account for variations in
recovery and instrument response. Mass spectrometric detection was carried out with a PE Sciex API III+ triple quadrupole mass spectrometer equipped with a Turbo IonSpray source as the LC-MS interface. Good intraday and interday assay precision (<10% CV) and accuracy (<10% difference) were observed over a concentration range of 0.005-2.5 μM in plasma.
The extraction recoveries were .apprx.90% and the method was found to be linear
for the assay (r2>0.999). The method has been successfully applied to discovery and preclin. pharmacokinetic studies, including a dose range-finding study and toxicokinetic exposure studies in rat and dog.

IT 292135-59-2, DPC 423
RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)
(development and validation of liquid chromatog.-mass spectrometric method for determination of DPC 423 in rat and dog plasma)

RN 292135-59-2 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 20 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

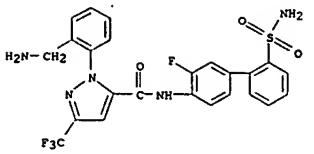
L9 ANSWER 21 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:84721 CAPLUS
DOCUMENT NUMBER: 139:255020
TITLE: Inhibition of factor Xa reduces ischemic brain damage after thromboembolic stroke in Rats
AUTHOR(S): Wang, Xinkang; Xu, Lin; Wang, Hugh; Grzanna, Reinhard; Zhan, Yutian; Knabb, Robert M.; Luettgen, Joseph M.; Bozarth, Tracy A.; Galemmo, Robert A.; Wong, Pancras C.; Bernard, Roberta; Vargas, Hugo; Chopp, Michael; Friedman, Steven M.; Feuerstein, Giora Z.
CORPORATE SOURCE: Departments of Cardiovascular Sciences, Neurosciences, General Pharmacology, and Medicinal Chemistry, Bristol-Myers Squibb Company, Wilmington, DE, USA
SOURCE: Stroke (2003), 34(2), 468-474
CODEN: SJCCA7; ISSN: 0039-2499
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Factor Xa (FXa) is a key coagulation protease and target for novel antithrombotic agents for prevention and treatment of diverse thromboembolic disorders. In the present study we describe the effect of a novel, potent, and selective FXa inhibitor, DPC602, on brain damage and neurobehavioral consequence in a rat thromboembolic model of stroke. Thromboembolic stroke was induced in rats by placement of an autologous clot into the middle cerebral artery. Laser-Doppler monitoring of cerebral blood flow demonstrated that DPC602 (8 mg/kg, single IV/IP bolus pretreatment) markedly improved cerebral blood flow after thromboembolic stroke by 25% to 160% (n = 6; P < 0.001) at 1 to 6 h. DPC602 demonstrated concentration- and time-dependent redns. in infarct size, with maximal effect (89% reduction; n = 14; P < 0.001) at the highest dose over controls. Neurol. function was also significantly improved in DPC602-treated rats at days 1, 3, and 7 (n = 13; P < 0.01). DPC602 treatment did not cause cerebral hemorrhage, assessed by free Hb in the ischemic brain tissues. These data suggest that anticoagulation with a selective FXa inhibitor might ameliorate the extent of ischemic brain damage and neurol. deficits after a thromboembolic event. Enhanced clot dissoln. and early reperfusion may account for the cerebrovascular-protective effect of the drug.

IT 228258-45-5, DPC602
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(factor Xa inhibitor DPC602 in ischemic brain damage after thromboembolic stroke)

RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 21 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

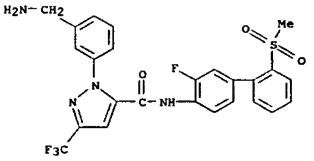
L9 ANSWER 22 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:932561 CAPLUS
DOCUMENT NUMBER: 138:378909
TITLE: Nonpeptide factor Xa inhibitors III: effects of DPC423, an orally-active pyrazole antithrombotic agent, on arterial thrombosis in rabbits
AUTHOR(S): Wong, Pancras C.; Crain, Earl J.; Watson, Carol A.; Zaspel, Alverna M.; Wright, Matthew R.; Lam, Patrick Y.; Pinto, Donald J. P.; Wexler, Ruth R.; Knabb, Robert M.
CORPORATE SOURCE: Cardiovascular Biology, Bristol-Myers Squibb Company, Wilmington, DE, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (2002), 303(3), 993-1000
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB DPC423 [1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide] is a synthetic, competitive, and selective inhibitor of coagulation factor Xa (fXa) (Ki: 0.15 nM in humans, 0.3 nM in rabbit). The objective of this study was to compare effects of DPC423, enoxaparin (low-mol.-weight heparin), and argatroban (thrombin inhibitor) on arterial thrombosis and hemostasis in rabbit models of elec. induced carotid artery thrombosis and cuticle bleeding, resp. Compds. were infused i.v. continuously from 60 min before artery injury or cuticle transection to the end of experiment Carotid blood flow was used as a marker of antithrombotic effect. Antithrombotic ED50 values were 0.4 mg/kg/h for enoxaparin (n = 6), 0.13 mg/kg/h for argatroban (n = 6), and 0.6 mg/kg/h for DPC423 (n = 12). DPC423 at the maximum antithrombotic dose increased activated partial thromboplastin time and prothrombin time (n = 6) by 1.8 ± 0.07- and 1.8 ± 0.13-fold, resp., without changes in thrombin time and ex vivo thrombin activity. The antithrombotic effect of DPC423 was significantly correlated with its ex vivo anti-fXa activity (r = 0.86). DPC423 at 1, 3, and 10 mg/kg p.o. increased carotid blood flow (percent control) at 45 min to 10 ± 4, 24 ± 6, and 74 ± 7, resp. (n = 6/group). Cuticle bleeding times (percent change over control) determined at the maximum antithrombotic dose were 88 ± 12 for argatroban, 69 ± 13 for heparin, 4 ± 3 for enoxaparin, 5 ± 4 for DPC423, and -3 ± 2 for the vehicle (n = 5-6/group), suggesting dissociation of antithrombotic and bleeding time effects for DPC423 and enoxaparin. The combination of aspirin and DPC423 at ineffective antithrombotic doses produced significant antithrombotic effect. Therefore, these results suggest that DPC423 is a clin. useful oral anticoagulant for the prevention of arterial thrombosis.

IT 292135-59-2, DPC423
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(factor Xa inhibitors: orally-active pyrazole antithrombotic agent DPC423)

RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 22 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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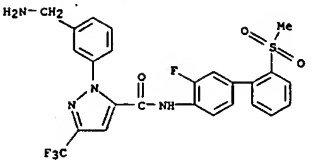
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 23 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:845163 CAPLUS
DOCUMENT NUMBER: 139:79
TITLE: Nonpeptide factor Xa inhibitors: DPC423, a highly potent and orally bioavailable pyrazole antithrombotic agent
AUTHOR(S): Wong, Pancras C.; Pinto, Donald J. P.; Knabb, Robert M.
CORPORATE SOURCE: Cardiovascular Biology, Bristol-Myers Squibb Company, Wilmington, DE, USA
SOURCE: Cardiovascular Drug Reviews (2002), 20(2), 137-152
CODEN: CDREEA; ISSN: 0897-5957
PUBLISHER: Neva Press
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. DPC 423 is a synthetic, orally bioavailable, competitive, and selective inhibitor of human coagulation factor Xa (Ki [nM]: factor Xa, 0.15; trypsin, 60; thrombin, 6000; plasma kallikrein, 61; activated protein C, 1800; factor IXa, 2200; factor VIIa, >15,000; chymotrypsin, >17,000; urokinase, >19,000; plasmin, >35,000; tissue plasminogen activator, >45,000; complement factor I, 44,000 [IC50]). In vitro, DPC 423 produced anticoagulant effects in human plasma in which it doubled prothrombin time, activated partial thromboplastin time, and Heptest clotting time at 3.1, 3.1, and 1.1 μM, resp. In dogs, DPC 423 had a good pharmacokinetic profile with an oral bioavailability of 57%, a plasma clearance of 0.24 L/kg/h, and a plasma half-life of 7.5 h. In rabbit and rat models of arteriovenous shunt thrombosis, DPC 423 was an effective antithrombotic agent with an IC50 of 150 and 470 nM, resp. The antithrombotic effect of DPC 423 is likely to be related to the inhibition of factor Xa but not to the inhibition of thrombin or due to direct inhibition of platelet aggregation. Therefore, based on potency, selectivity, efficacy, and oral bioavailability, DPC 423 was selected for clin. development as an oral anticoagulant for the potential treatment of thrombotic disorders. Preliminary human data suggest that DPC 423 is orally bioavailable in humans and has a long plasma half-life.
IT 292135-59-2, DPC 423
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(DPC 423 as factor Xa inhibitor and highly potent and orally bioavailable antithrombotic agent)
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 23 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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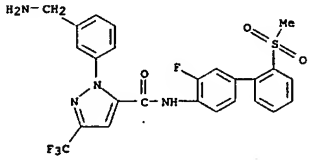
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 24 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:621918 CAPLUS
DOCUMENT NUMBER: 138:147036
TITLE: DPC-423 (Bristol-Myers squibb)
AUTHOR(S): Taglialatela, Maurizio
CORPORATE SOURCE: Section of Pharmacology, Department of Neuroscience, University of Naples "Federico II", Naples, 80131, Italy
SOURCE: Current Opinion in Investigational Drugs (PharmaPress Ltd.) (2002), 3(2), 252-254
CODEN: COIDAZ; ISSN: 1472-4472
PUBLISHER: PharmaPress Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. DPC-423 is a biphenylamine-containing amide which is under development by Bristol-Myers Squibb (formerly DuPont Pharmaceuticals) as a Factor Xa inhibitor for the potential treatment of thrombotic disorders. As of August 2000, DPC-423 was in phase I trials. DPC-423 was discovered as a result of SAR modifications of DuPont's SN-429, including replacement of the benzamidine moiety with a less basic benzylamine. Its 2-aminomethylphenyl analog DPC-602 is also under investigation for thrombotic disorders.
IT 292135-59-2, DPC-423
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(DPC-423 a factor Xa inhibitor).
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

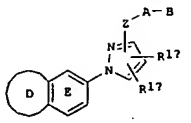
L9 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:39605 CAPLUS
DOCUMENT NUMBER: 136:102380
TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John M.; Han, Qi; Li, Renhua; Pinto, Donald J. P.; Pruitt, James R.; Quan, Mimi L.
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA
SOURCE: U.S., 117 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 6339099 | B1 | 20020115 | US 1998-99358 | 19980618 |
| US 2002025963 | A1 | 20020228 | US 2001-924381 | 20010808 |
| US 6906070 | B2 | 20050614 | | |
| US 2003069258 | A1 | 20030410 | US 2002-98994 | 20020313 |
| US 6958356 | B2 | 20051025 | | |
| US 2004063772 | A1 | 20040401 | US 2003-602214 | 20030624 |
| US 6965036 | B2 | 20051115 | | |
| US 2006040973 | A1 | 20060223 | US 2005-197978 | 20050805 |

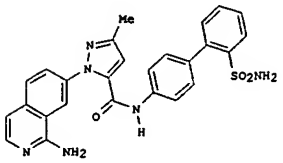
PRIORITY APPLN. INFO.: US 1997-50265P P 19970620
US 1998-99358 A3 19980618
US 2001-924381 B1 20010808
US 2002-98994 A1 20020313

OTHER SOURCE(S): MARPAT 136:102380
GI

L9 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



II

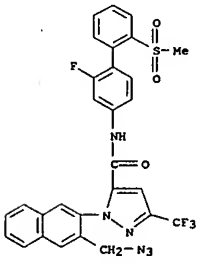


II

AB The title compds. [I; ring D = 5-membered aromatic system containing from 1-2
heteroatoms selected from N, O, S; ring D is substituted with 0-2 R groups; ring E contains 0-2 N atom and is substituted by 0-1 R groups; R =
Cl, F, Br, I, OH, alkoxy, amino(alkyl), (alkyl)amino; Z = bond, alkylene, (CH2)rO(CH2)r, (CH2)rNR3(CH2)r, (CH2)rC(O)(CH2)r, (CH2)rC(O)O(CH2)r, (CH2)rOC(O)(CH2)r, (CH2)rC(O)NR3(CH2)r, etc. provided that Z does not form
a N-N, N-O, N-S, NCH2N, NCH2O, or NCH2S bond with ring M or group A; R1a-1b = H, alk(en)yl, aminoalkyl, alkoxy, alternatively, R1a-1b, when attached to adjacent carbon atoms, together with the atoms to which they are attached form a 5-8 membered (un)saturated ring (un)substituted and which
contains from 0-2 heteroatoms selected from the group consisting of N, O, and S; alternatively, when Z is C(O)NH and R1a is attached to a ring carbon adjacent to Z, then R1a is a C(O) which replaces the amide hydrogen
of Z to form a cyclic imide; R3 = H, alkyl, phenyl; A = (un)substituted carbocyclic, 5-10 membered heterocyclic system containing 1-4 heteroatoms selected from N, O, S; B = H, Y, X-Y; X = sulfonylalkyl, alkylsulfonyl, sulfonamide, etc.; Y = alkylamino, provided that X-Y does not form a N-N, O-N or S-N bond, carbocyclic group, 5-10 membered heterocyclic r = 0-3], inhibitors of factor Xa which are useful in treating and preventing a thromboembolic disorder, were prepared and formulated. Thus, a multi-step
synthesis of the title compound II, starting with 7-aminoisoquinoline, was
described. A number of compds. I were found to exhibit a Ki of ≤ 15 μM against factor Xa.

IT 218299-04-8P

L9 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



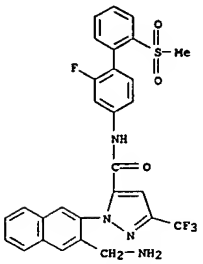
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of novel guanidine mimics as factor Xa inhibitors)

RN 218299-04-8 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-2-naphthalenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT 218302-16-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel guanidine mimics as factor Xa inhibitors)

RN 218302-16-0 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(azidomethyl)-2-naphthalenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:881167 CAPLUS

DOCUMENT NUMBER: 136:160835

TITLE: Disposition of 1-[3-(Aminomethyl)phenyl]-N-[3-fluoro-2'- (methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- 1H-pyrazole-5-carboxamide (DPC 423)
by Novel Metabolic Pathways. Characterization of Unusual Metabolites by Liquid Chromatography/Mass Spectrometry and NMR

AUTHOR(S): Mutlib, Abdul. E.; Shockcor, John; Chen, Shiang-Yuan; Espina, Robert J.; Pinto, Donald J.; Orwat, Michael J.; Prakash, Shimoga R.; Gan, Liang-Shang

CORPORATE SOURCE: Stine-Haskell Research Center, Drug Metabolism and Pharmacokinetics Section, DuPont Pharmaceuticals Company, Newark, DE, 19714, USA

SOURCE: Chemical Research in Toxicology (2002), 15(1), 48-62
CODEN: CRTOEC; ISSN: 0893-228X

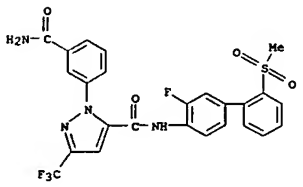
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The in vitro and in vivo disposition of DPC 423 was investigated in mice, rats, dogs and humans and the metabolites characterized by LC/MS, LC/NMR and high field-NMR. The rodents produced several metabolites that included an aldehyde (M1), a carboxylic acid (M2), a benzyl alc. (M3), glutamate conjugates (M4 and M5), an acyl glucuronide (M6) and its isomers; a carbamyl glucuronide (M7); a phenol (M8) and its glucuronide conjugate (M9), two glutathione adducts (M10 and M11), a sulfamate conjugate (M12), isomers of an oxime metabolite (M13), and an amide (M14).
Humans and dogs produced less complex metabolite profiles than rats. While unchanged DPC 423 was the major component in plasma and urine samples, differences in the metabolic disposition of this compound among species were noted. M1 is believed to be rapidly oxidized to the carboxylic acid (M2), which forms the potentially reactive acyl glucuronide (M6). The formation of novel glutamate conjugates (M4 and M5)
and their role in depleting endogenous glutathione have been described previously. The carbamyl glucuronide M7, found as the major metabolite in
rats and in other species, was considered nonreactive and was easily hydrolyzed to the parent compound in the presence of β-glucuronidase. The identification of GSH adducts M10 and M11 led us to postulate the existence of at least two reactive intermediates responsible for their formation, an epoxide and possibly a nitrile oxide, resp. Although the formation of GSH adducts such as M10 from epoxides has been described before, there are no reports to date describing the existence of a GSH adduct (M11) of an oxime. The formation of a sulfamate conjugate (M12) formed by direct coupling of sulfate to the nitrogen of benzylamine is described. A mechanism is proposed for the formation of the oxime (M13) that involves sequential oxidation of the benzylamine to the corresponding
hydroxylamine and nitroso intermediate. The rearrangement of the nitroso intermediate is believed to produce the oxime (M13). In vitro studies suggested that both the oxime (M13) and the aldehyde (M1) were precursors to the carboxylic acid (M2). This is the first demonstration of carboxylic acid formation via an oxime intermediate produced from an amine. The stability of DPC423 in plasma obtained from several species was studied. Significant species differences in the plasma stability of DPC 423 were observed The formation of the aldehyde metabolite (M1) was

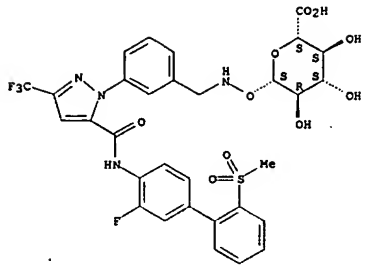
L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
found to be catalyzed by a semicarbazide-sensitive monoamine oxidase (SSAO) found in plasma of rabbits, dogs, and rhesus monkeys. Rat, chimpanzee, and human plasma did not form M1.
IT 395095-29-1 395095-30-4 397249-90-0
397249-91-1 397249-93-3 397249-94-4
397249-95-5 397249-96-6 397249-97-7
RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)
(disposition of DPC 423 by novel metabolic pathways and characterization of unusual metabolites by liquid chromatog./mass spectrometry and NMR)
RN 395095-29-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 395095-30-4 CAPLUS
CN β-D-Glucopyranuronic acid, 1-O-[[[3-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

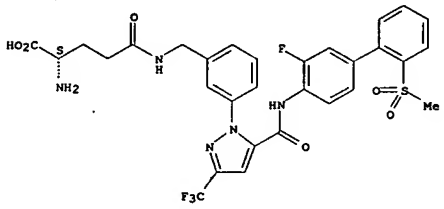
Absolute stereochemistry.

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 397249-90-0 CAPLUS
CN L-Glutamine, N-[[3-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]- (9CI) (CA INDEX NAME)

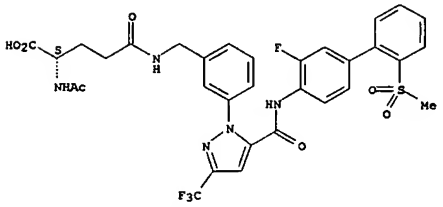
Absolute stereochemistry.



RN 397249-91-1 CAPLUS
CN L-Glutamine, N2-acetyl-N-[[3-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]- (9CI) (CA INDEX NAME)

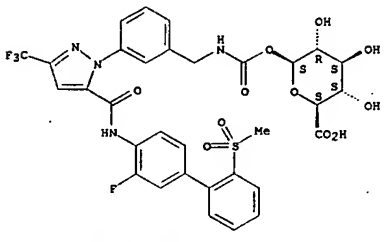
Absolute stereochemistry.

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



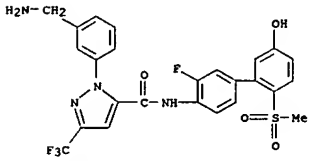
RN 397249-93-3 CAPLUS
CN β-D-Glucopyranuronic acid, 1-[[[3-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]carbamate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



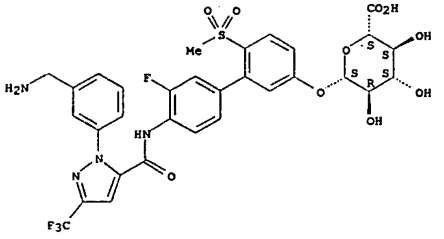
RN 397249-94-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-5'-hydroxy-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 397249-95-5 CAPLUS
CN β-D-Glucopyranosiduronic acid, 4'-[[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-3'-fluoro-6-(methylsulfonyl)[1,1'-biphenyl]-3-yl (9CI) (CA INDEX NAME)

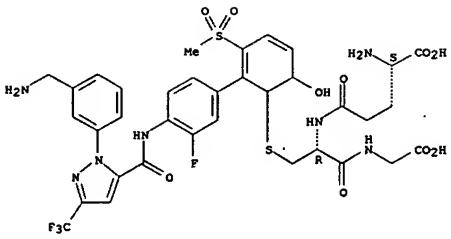
Absolute stereochemistry.



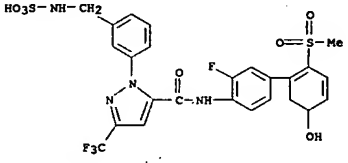
RN 397249-96-6 CAPLUS
CN Glycine, L-γ-glutamyl-S-[2-[4-[[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-3-fluorophenyl]-6-hydroxy-3-(methylsulfonyl)-2,4-cyclohexadien-1-yl]-L-cysteinyl- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

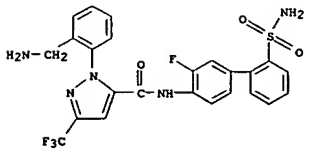


RN 397249-97-7 CAPLUS
CN Sulfamic acid, [[3-[5-[[[2-fluoro-4-[5-hydroxy-2-(methylsulfonyl)-1,3-cyclohexadien-1-yl]phenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]- (9CI) (CA INDEX NAME)

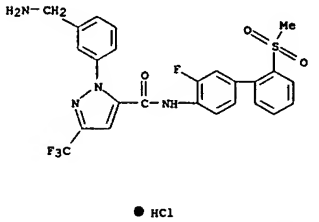


IT 228258-45-5, DPC 602 292135-59-2, DPC 423
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(disposition of DPC 423 by novel metabolic pathways and characterization of unusual metabolites by liquid chromatog./mass spectrometry and NMR)
RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

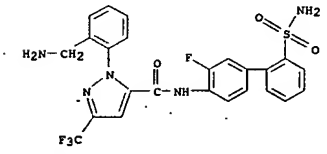


REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

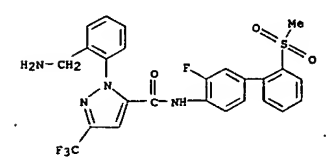
L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:881166 CAPLUS
DOCUMENT NUMBER: 136:144634
TITLE: P450-mediated metabolism of 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole- 5-carboxamide (DPC 423) and its analogs to aldoximes. Characterization of glutathione conjugates of postulated intermediates derived from aldoximes
AUTHOR(S): Mutlib, Abdul E.; Chen, Shiang-Yuan; Espina, Robert J.; Shockcor, John; Prakash, Shimoga R.; Gan, Liang-Shang
CORPORATE SOURCE: Stine-Haskell Research Center, Drug Metabolism and Pharmacokinetics Section, DuPont Pharmaceuticals Company, Newark, DE, 19714, USA
SOURCE: Chemical Research in Toxicology (2002), 15(1), 63-75
CODEN: CRTOEC; ISSN: 0893-228X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The in vivo and in vitro disposition of DPC 423, a highly potent, selective, and orally bioavailable inhibitor of blood coagulation factor Xa, has recently been described. Several metabolites, some of which were considered potentially reactive, were identified in rats. A novel GSH adduct, the structure of which was not determined conclusively, was isolated from bile of rats dosed with DPC 423. Herein, we describe the complete structural elucidation of this unique GSH conjugate employing LC/MS and high-field NMR. Similar GSH adducts of DPC 602, [13CD2]DPC 602, and SX 737, all structural analogs of DPC 423, were isolated, characterized spectroscopically, and shown to have identical mass fragmentation pathways. The structures of these conjugates were initially suspected to be either an amide with N-S bond or a nitrogen-oxygen juxtaposed amide with a C-S bond. Studies conducted with [13CD2]DPC 602 indicated an aldoxime structure. The concluding evidence came from HMBC NMR spectrum of the conjugate, which showed strong correlation of the cysteine methylene protons with the imino carbon. Further spectroscopic studies with chemical prepared GSH adduct from benzaldehyde oxime confirmed this pattern of correlation. In vivo and in vitro studies with the synthetic oxime intermediate from DPC 423 showed an adduct identical to the one isolated from the bile of rats dosed with DPC 423. This supported the intermediacy of an aldoxime as a precursor to the GSH adducts. It is postulated that the benzylamine moiety of DPC 423 (and its analogs) is oxidized to a hydroxylamine, which is subsequently converted to a nitroso intermediate. Subsequent rearrangement of the nitroso leads to an aldoxime which in turn is metabolized by P 450 to a reactive intermediate.
The formation of oxime from DPC 423 (and its analogs) was found to be mediated by rat CYP 3A1/2, which were also responsible for converting the oxime to the GSH trappable reactive intermediate. It is postulated that the aldoxime produces a radical or a nitrile oxide intermediate that reacts with GSH and hence produces this unusual GSH adduct. On the basis of synthetic analogy, it is more likely that the nitrile oxide resulting from two-electron oxidation of the aldoxime is the reactive intermediate. Intramol. kinetic isotope effects were studied with [13CD2]DPC 602 to assess the importance of the metabolic cleavage of the aminomethyl carbon-hydrogen bond in forming this GSH adduct. The lack of isotope

L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
effect in forming the aldoxime from [13CD2]DPC 602 suggests its formation does not occur through the imine intermediate. Instead the data supports the postulated mechanism of hydroxylamine and nitroso intermediates as precursors to the aldoxime. However, the formation of the GSH adduct from [13CD2]DPC 602 did show a significant intramol. kinetic isotope effect (kH/kD = 2.3) since a carbon-deuterium bond had to be broken on the aldoxime prior to the formation of the adduct. A stable nitrile oxide derived from DPC 602 was postulated as the reactive intermediate responsible for forming this unique GSH adduct.
IT 228258-45-5P, DPC 602 228258-46-6P, SX 737 292135-59-2P, DPC 423 395095-27-9P 395095-29-1P 395095-30-4P 395095-32-6P 395685-16-2P, [13CD2]DPC 602
RL: PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(P 450-mediated metabolism of blood coagulation factor Xa inhibitor DPC 423 and its analogs to aldoximes: characterization of glutathione conjugates)
RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

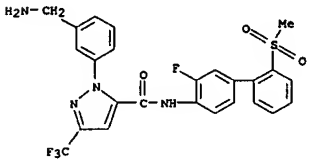


RN 228258-46-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



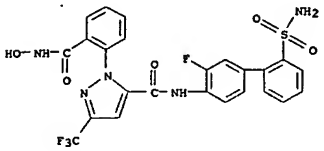
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-

L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



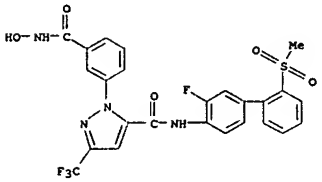
● HCl

RN 395095-27-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-1-[2-[(hydroxyamino)carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

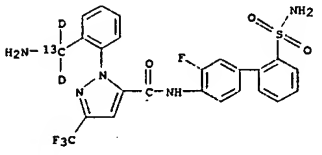


RN 395095-29-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

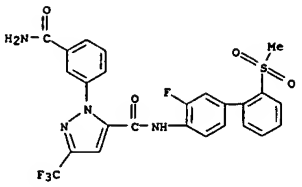


RN 395685-16-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl-13C-d2)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



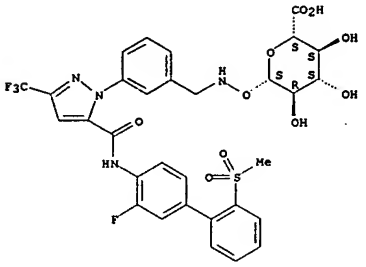
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 395095-30-4 CAPLUS
CN β-D-Glucopyranuronic acid, 1-O-[[[3-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 395095-32-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[3-[(hydroxyamino)carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

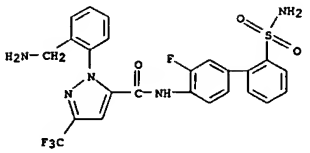
ACCESSION NUMBER: 2001:705983 CAPLUS
DOCUMENT NUMBER: 136:79226
TITLE: Formation of unusual glutamate conjugates of 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC 423) and its analogs: the role of γ-glutamyltranspeptidase in the biotransformation of benzylamines
AUTHOR(S): Mutlib, Abdul; Shockcor, John; Chen, Shiang-Yuan; Espina, Robert; Lin, Jianrong; Graciani, Nilsa; Prakash, Shimoga; Gan, Liang-Shang
CORPORATE SOURCE: Drug Metabolism and Pharmacokinetics Section, Stine-Haskell Research Center, DuPont Pharmaceuticals Company, Newark, DE, 19714, USA
SOURCE: Drug Metabolism and Disposition (2001), 29(10), 1296-1306
CODEN: DMDSAI; ISSN: 0090-9556
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The role of γ-glutamyltranspeptidase (GGT) in transferring glutamate from endogenous glutathione (GSH) to the benzylamine moiety of a compound, such as 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC 423), is described. Studies were performed with structurally related analogs of DPC 423 to demonstrate that this type of reaction was common to compds. possessing a benzylamine group. Synthesizing appropriate stds. and confirming by liquid chromatog. (LC)/mass spectroscopy and LC/NMR made unambiguous assignments of the structures of glutamate conjugates of DPC 423. The use of stable isotope-labeled GSH for metabolism studies has not been described before. In the present study, we report the novel use of deuterated GSH in conjunction with mass spectral anal. to demonstrate the glutamate transfer to the benzylamines in the presence of GGT. To further demonstrate that the α protons on the benzylamines and glutamate (as part of glutathione) were unaffected during the transpeptidation, these protons were replaced with deuterium. Acivicin (AT-125), a potent and selective inhibitor of GGT, was used to abolish the formation of the glutamate conjugates of DPC 423 in vitro and in vivo. This provided further evidence of the role of GGT in forming the glutamate conjugates of benzylamines. This study demonstrated conclusively that GGT was responsible for mediating the transfer of glutamic acid from GSH to the benzylamine moiety of a series of structurally related compds.

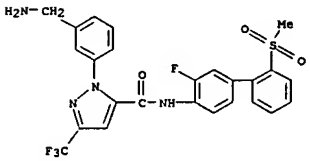
IT 228258-45-5 292135-59-2, DPC 423 292135-59-2D, DPC 423, glutamate conjugates
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(formation of unusual glutamate conjugates of DPC 423 and its analogs and role of γ-glutamyltranspeptidase in the biotransformation of benzylamines)

RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



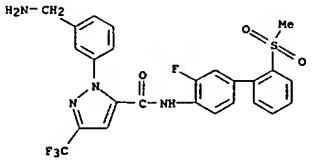
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

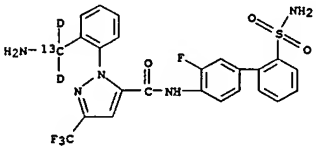
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

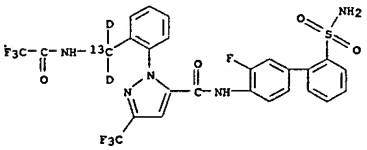
IT 385380-71-2P
RL: PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(formation of unusual glutamate conjugates of DPC 423 and its analogs and role of γ-glutamyltranspeptidase in the biotransformation of benzylamines)
RN 385380-71-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl-13C-d2)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 385380-68-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(formation of unusual glutamate conjugates of DPC 423 and its analogs and role of γ-glutamyltranspeptidase in the biotransformation of benzylamines)
RN 385380-68-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-

L9 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
yl]-1-[2-[[(trifluoroacetyl)amino]methyl-13C-d2]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



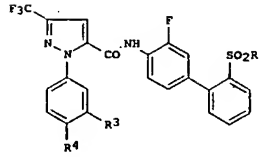
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

| | |
|---|---|
| ACCESSION NUMBER: | 2001:300687 CAPLUS |
| DOCUMENT NUMBER: | 134:311206 |
| TITLE: | Preparation of 1,3,5-trisubstituted pyrazoles for pharmaceutical use as factor Xa inhibitors |
| INVENTOR(S): | Zhou, Jiacheng; Oh, Lynette May; Confalone, Pasquale N.; Li, Hui-yin; Ma, Philip |
| PATENT ASSIGNEE(S): | Du Pont Pharmaceuticals Company, USA |
| SOURCE: | PCT Int. Appl., 103 pp.<br>CODEN: PIXXD2 |
| DOCUMENT TYPE: | Patent |
| LANGUAGE: | English |
| FAMILY ACC. NUM. COUNT: | 1 |
| PATENT INFORMATION: | |

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001029006 | A1 | 20010426 | WO 2000-US29031 | 20001020 |
| W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| US 6329527 | B1 | 20011211 | US 2000-685127 | 20001010 |
| CA 2382212 | A1 | 20010426 | CA 2000-2382212 | 20001020 |
| EP 1222172 | A1 | 20020717 | EP 2000-972292 | 20001020 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY | | | | |
| US 2002055641 | A1 | 20020509 | US 2001-5938 | 20011203 |
| US 6465656 | B2 | 20021015 | | |
| PRIORITY APPLN. INFO.: | | | US 1999-161666P | P 19991021 |
| | | | US 2000-685127 | A3 20001010 |
| | | | WO 2000-US29031 | W 20001020 |

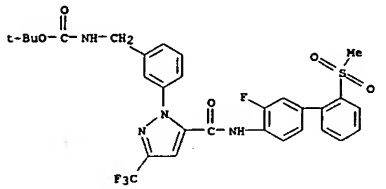
OTHER SOURCE(S): MARPAT 134:311206
GI



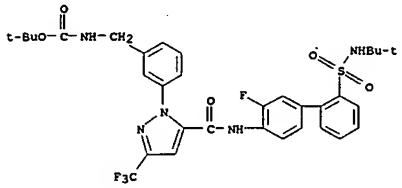
I

AB 1,3,5-Trisubstituted pyrazoles, such as I [R = Me, NH2; R3 = CN, CH2NH2; R4 = H, F], were prepared for pharmaceutical use as factor Xa inhibitors (no biol. testing data presented). Thus, I (R = Me, R3 = CN, R4 = H) was

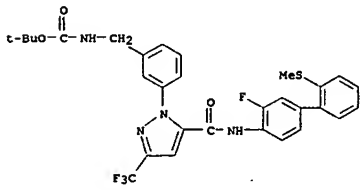
L9 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
prepd. via cyclization of F3CCONHNHC6H4-3-CN with H2C:CHCONHC6H3(-2-F)-4-C6H4-2-SO2Me and subsequent dehydrogenation of the resulting pyrazoline using N-chlorosuccinimide.
IT 335275-82-6P 335275-91-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 1,3,5-trisubstituted pyrazoles for pharmaceutical use as
factor Xa inhibitors)
RN 335275-82-6 CAPLUS
CN Carbamic acid, [[3-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



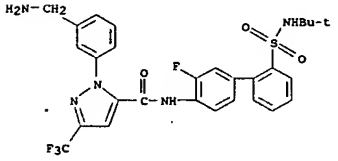
RN 335275-91-7 CAPLUS
CN Carbamic acid, [[3-[5-[[[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN Carbamic acid, [[3-[5-[[[3-fluoro-2'-(methylthio)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



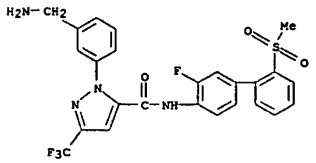
RN 335275-92-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

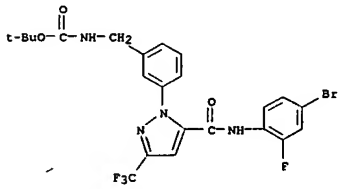
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 292135-59-2P 335275-89-3P 335275-90-6P
335275-92-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,3,5-trisubstituted pyrazoles for pharmaceutical use as
factor Xa inhibitors)
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 335275-89-3 CAPLUS
CN Carbamic acid, [[3-[5-[[(4-bromo-2-fluorophenyl)amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester
(9CI) (CA INDEX NAME)



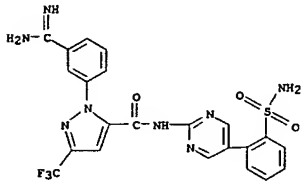
RN 335275-90-6 CAPLUS

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:55833 CAPLUS
DOCUMENT NUMBER: 134:246871
TITLE: Discovery of 1-[3-(Aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC423), a Highly Potent, Selective, and Orally Bioavailable Inhibitor of Blood Coagulation Factor Xa
AUTHOR(S): Pinto, Donald J. P.; Orwat, Michael J.; Wang, Shuaige; Fevig, John M.; Quan, Mimi L.; Amparo, Eugene; Cacciola, Joseph; Rossi, Karen A.; Alexander, Richard S.; Smallwood, Angela M.; Luettgen, Joseph M.; Liang, Li; Aungst, Bruce J.; Wright, Matthew R.; Knabb, Robert M.; Wong, Pancras C.; Wexler, Ruth R.; Lam, Patrick Y. S.
CORPORATE SOURCE: DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(4), 566-578
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:246871
AB Factor Xa (fXa) plays a critical role in the coagulation cascade, serving as
the point of convergence of the intrinsic and extrinsic pathways. Together with nonenzymic cofactor Va and Ca2+ on the phospholipid surface of platelets or endothelial cells, factor Xa forms the prothrombinase complex, which is responsible for the proteolysis of prothrombin to catalytically active thrombin. Thrombin, in turn, catalyzes the cleavage of fibrinogen to fibrin, thus initiating a process that ultimately leads to clot formation. Recently, the authors reported on a series of isoxazoline and isoxazole monobasic noncovalent inhibitors of factor Xa which show good potency in animal models of thrombosis. In this paper, the authors wish to report on the optimization of the heterocyclic core, which ultimately led to the discovery of a novel pyrazole SN429 (fXa Ki = 13 pM). The authors also report on the authors efforts to improve the oral bioavailability and pharmacokinetic profile of this series while maintaining subnanomolar potency and in vitro selectivity. This was achieved by replacing the highly basic benzamidine P1 with a less basic benzylamine moiety. Further optimization of the pyrazole core substitution and the biphenyl P4 culminated in the discovery of DPC423, a highly potent, selective, and orally active factor Xa inhibitor which was chosen for clin. development.
IT 209955-39-5P 209955-61-3P 209957-34-6P
209957-36-8P 209957-48-2P 209957-52-8P
292135-59-2P, DPC 423
RL: BAC (Biological activity or effector, except adverse); BPR (Biological
process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(discovery of pyrazolecarboxamide derivative (DPC423) as a highly potent
and orally bioavailable inhibitor of blood coagulation factor Xa with good pharmacokinetics and structure-activity relationships)
RN 209955-39-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(aminosulfonyl)phenyl]-2-pyrimidinyl}-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-38-4
CMF C22 H17 F3 N8 O3 S



CM 2

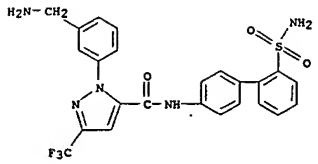
CRN 76-05-1
CMF C2 H F3 O2

RN 209955-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-
(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-60-2
CMF C24 H20 F3 N5 O3 S

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



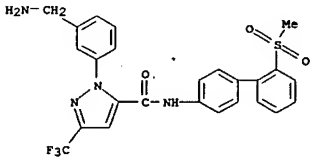
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-34-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-(2'-
(methylsulfonyl)[1,1'-biphenyl]-4-yl}-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-33-5
CMF C25 H21 F3 N4 O3 S



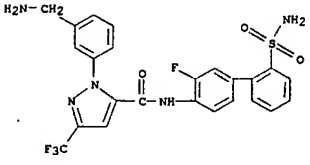
CM 2

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 76-05-1
CMF C2 H F3 O2

RN 209957-36-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-
3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
mono(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM 1

CRN 209957-35-7
CMF C24 H19 F4 N5 O3 S



CM 2

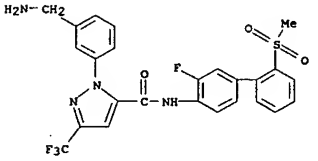
CRN 76-05-1
CMF C2 H F3 O2

RN 209957-48-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-{3-(aminomethyl)phenyl]-N-{3-fluoro-2'-
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-47-1

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C25 H20 F4 N4 O3 S



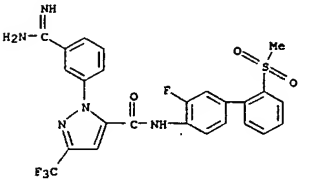
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-52-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

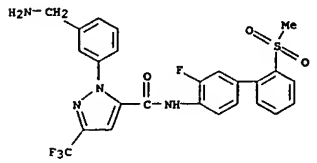
CRN 209957-51-7
CMF C25 H19 F4 N5 O3 S



CM 2

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 76-05-1
CMF C2 H F3 O2

RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 209954-60-9P 209955-28-2P 209957-54-0P
331006-14-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(discovery of pyrazolecarboxamide derivative (DPC423) as a highly potent and orally bioavailable inhibitor of blood coagulation factor Xa with good pharmacokinetics and structure-activity relationships)
RN 209954-60-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-59-6
CMF C24 H19 F3 N6 O3 S

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

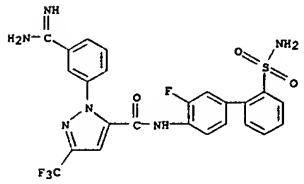
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-54-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-53-9
CMF C24 H18 F4 N6 O3 S

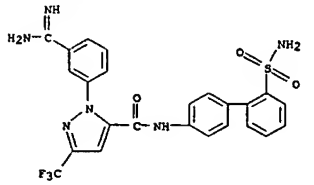


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 331006-14-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



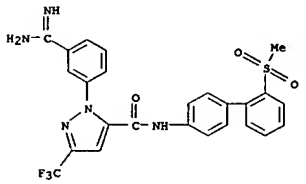
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-28-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

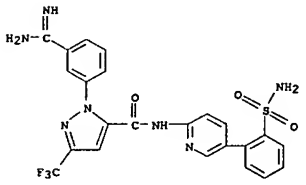
CM 1

CRN 209954-94-9
CMF C25 H20 F3 N5 O3 S



L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CM 1

CRN 209955-48-6
CMF C23 H18 F3 N7 O3 S

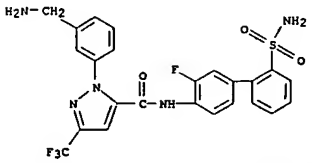


CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 209957-35-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(discovery of pyrazolecarboxamide derivative (DPC423) as a highly potent and orally bioavailable inhibitor of blood coagulation factor Xa with good pharmacokinetics and structure-activity relationships)
RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

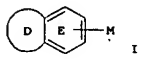
L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:725629 CAPLUS
DOCUMENT NUMBER: 133:296430
TITLE: Preparation of aryl sulfonyls as factor Xa inhibitors
INVENTOR(S): Wexler, Ruth R.; Jacobson, Irina C.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000059902 | A2 | 20001012 | WO 2000-US8364 | 20000330 |
| WO 2000059902 | A3 | 20010426 | | |
| W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| CA 2368630 | A1 | 20001012 | CA 2000-2368630 | 20000330 |
| EP 1175419 | A2 | 20020130 | EP 2000-923096 | 20000330 |
| EP 1175419 | B1 | 20030528 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| AT 241621 | T | 20030615 | AT 2000-923096 | 20000330 |
| ES 2197092 | T3 | 20040101 | ES 2000-923096 | 20000330 |
| US 6399644 | B1 | 20020604 | US 2000-540467 | 20000331 |
| US 2003050315 | A1 | 20030313 | US 2002-74301 | 20020212 |
| US 6689770 | B2 | 20040210 | | |

| | | | |
|---|---|---|---|
| PRIORITY APPLN. INFO.: | US 1999-127634P | P | 19990402 |
| | WO 2000-US8364 | W | 20000330 |
| | US 2000-540467 | A3 | 20000331 |

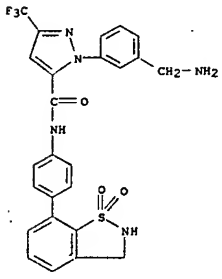
OTHER SOURCE(S): MARPAT 133:296430
GI



I

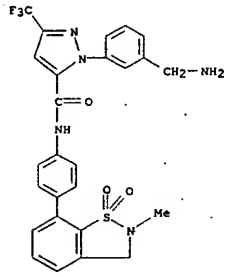
AB Aryl sulfonyls I [ring D is absent or is CH2N:CH, CH:NCH2, aromatic system
containing heteroatoms, etc.; E = Ph, pyridyl, pyrazinyl, etc.; M = heterocyclyl], effective factor Xa inhibitors (no data), were prepared E.g., N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-1-(4-

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide was prepd.
IT 300710-16-1P 300710-17-2P 300710-18-3P
300710-21-8P 300710-22-9P 300710-23-0P
300710-24-1P 300710-28-5P 300710-33-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl sulfonyls as factor Xa inhibitors)
RN 300710-16-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

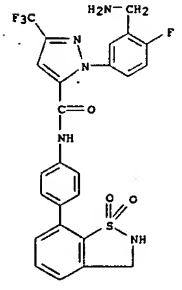


RN 300710-17-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

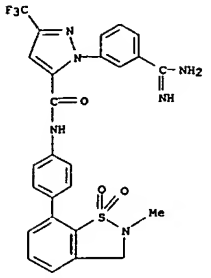


RN 300710-18-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

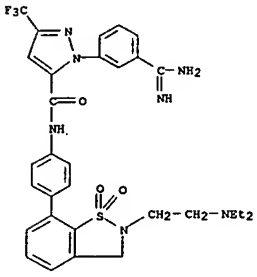


RN 300710-21-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

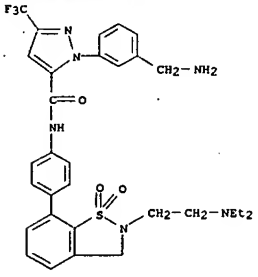


RN 300710-22-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-[2-[2-(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

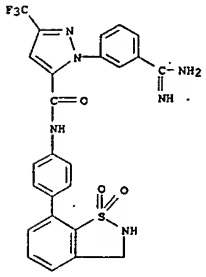


RN 300710-23-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxidobenzo[b]thien-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

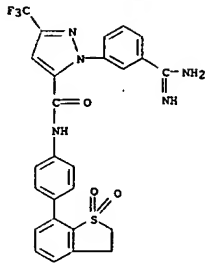


RN 300710-33-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

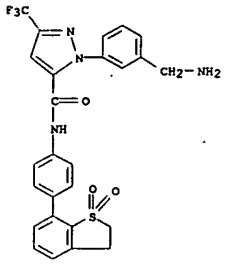


IT 300710-45-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl sulfonyls as factor Xa inhibitors)
RN 300710-45-6 CAPLUS
CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

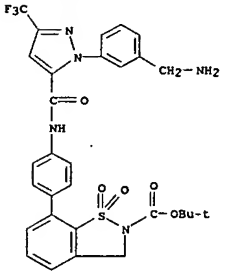


RN 300710-24-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxidobenzo[b]thien-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 300710-28-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[2-[2-(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

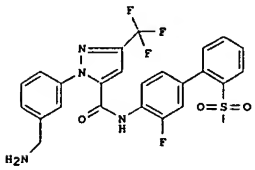
L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L9 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:645898 CAPLUS
DOCUMENT NUMBER: 133:232835
TITLE: Treatment of thrombosis by combined use of a factor xa inhibitor and aspirin, tissue plasminogen activator (TPA), a GPIIb/IIIa antagonist, low molecular weight heparin or heparin
INVENTOR(S): Wong, Pancras C.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000053264 | A1 | 20000914 | WO 2000-US6451 | 20000310 |
| W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| US 6794412 | B1 | 20040921 | US 2000-519188 | 20000306 |
| CA 2361650 | A1 | 20000914 | CA 2000-2361650 | 20000310 |
| EP 1161279 | A1 | 20011212 | EP 2000-913894 | 20000310 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| BR 2000010381 | A | 20020205 | BR 2000-10381 | 20000310 |
| AU 766089 | B2 | 20031009 | AU 2000-35254 | 20000310 |
| NZ 513217 | A | 20031128 | NZ 2000-513217 | 20000310 |
| ZA 2001006360 | A | 20020802 | ZA 2001-6360 | 20010802 |
| PRIORITY APPLN. INFO.: | | | US 1999-123815P | P 19990311 |
| | | | WO 2000-US6451 | W 20000310 |

GI

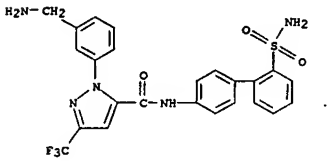


I

L9 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
AB Provided is a method of treating thrombosis in mammals by administering therapeutically effective amts. of a combination of (i) a Factor Xa inhibitor, and (ii) a compound selected from the group consisting of aspirin, TPA, a GPIIb/IIIa antagonist, low mol. weight heparin and heparin, wherein the dose administered for at least one of (i) and (ii) is a subtherapeutic dose. Preferably, the combination of (i) and (ii) provides a synergistic effect. A combination of I (Factor Xa inhibitor) and aspirin at their subtherapeutic doses produced a significant antithrombotic effect in a rabbit model of arterial thrombosis. Pharmaceutical dosage forms are discussed.
IT 209955-61-3 209957-48-2 292135-59-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(antithrombotic combination of a Factor Xa inhibitor and aspirin, TPA, a GPIIb/IIIa antagonist, or heparin derivative)
RN 209955-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-60-2
CMF C24 H20 F3 N5 O3 S



CM 2

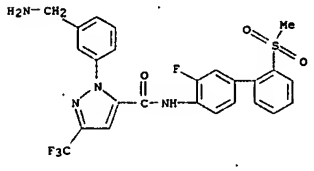
CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209957-48-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-47-1
CMF C25 H20 F4 N4 O3 S

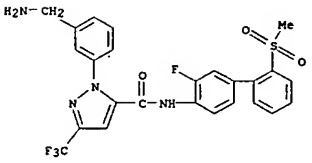


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



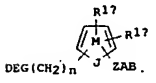
● HCl

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:83115 CAPLUS
DOCUMENT NUMBER: 132:137392
TITLE: Preparation of azoles as Factor Xa inhibitors.
INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell; Cacciola, Joseph; Fevig, John Matthew; Han, Qi; Orwat, Michael James; Quan, Mimi Lifen; Rossi, Karen Anita
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Co., USA
SOURCE: U.S., 152 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

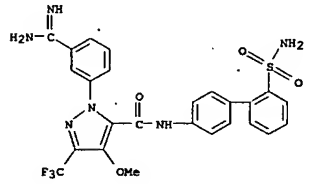
| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|
| US 6020357 | A | 20000201 | US 1997-995834 | | 19971222 |
| US 6548512 | B1 | 20030415 | US 2000-492708 | | 20000127 |
| PRIORITY APPLN. INFO.: | | | US 1996-33437P | P | 19961223 |
| | | | US 1997-50304P | P | 19970620 |
| | | | US 1997-995834 | A3 | 19971222 |

OTHER SOURCE(S): MARPAT 132:137392
GI



AB Title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(:NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = C1-4 alkylene, (CH2)rO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2; with provisos], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the

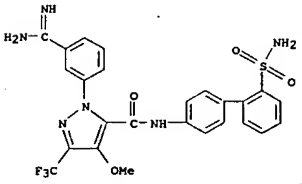
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Pinner reaction of the resulting intermediate afforded 1-(3-amidinophenyl)-2-{(2'-aminosulfonyl-1,1'-biphen-4-yl)aminocarbonyl}imidazole. Several I showed Ki ≤10 μM against Factor Xa and thrombin.
IT 209954-61-0P 209954-62-1P 209954-94-9P
209954-95-0P 209954-96-1P 209955-26-0P
209955-27-1P 209955-28-2P 209955-37-3P
209955-41-9P 209955-44-2P 209955-45-3P
209955-46-4P 209955-47-5P 209955-48-6P
209955-49-7P 209955-50-0P 209955-51-1P
209955-52-2P 209955-53-3P 209955-60-2P
209955-61-3P 209956-54-7P 209956-70-7P
209956-75-2P 209956-76-3P 209956-77-4P
209956-78-5P 209956-99-0P 209957-00-6P
209957-27-7P 209957-28-8P 209957-29-9P
209957-30-2P 209957-31-3P 209957-32-4P
209957-33-5P 209957-34-6P 209957-35-7P
209957-36-8P 209957-38-0P 209957-40-4P
209957-41-5P 209957-42-6P 209957-47-1P
209957-48-2P 209957-50-6P 209957-51-7P
209957-52-8P 209957-53-9P 209957-54-0P
209957-67-5P 209957-68-6P 209957-73-3P
209957-74-4P 209957-83-5P 209957-89-1P
209957-90-4P 209957-91-5P 209957-92-6P
209957-93-7P 209958-13-4P 209958-14-5P
209958-21-4P 209958-22-5P 209958-28-1P
209958-29-2P 209958-30-5P 209958-31-6P
209958-33-8P 256512-05-7P 256512-19-3P
256512-30-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azoles as Factor Xa inhibitors)
RN 209954-61-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-4-methoxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 209954-62-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-4-methoxy-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-61-0
CMF C25 H21 F3 N6 O4 S

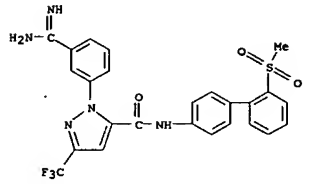


CM 2

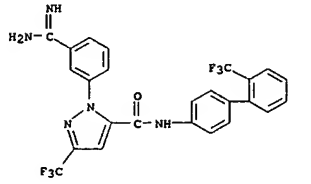
CRN 76-05-1
CMF C2 H F3 O2

RN 209954-94-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

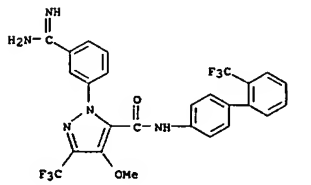
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209954-95-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 209954-96-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-4-methoxy-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

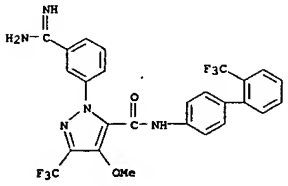


L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209955-26-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-4-methoxy-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-96-1
CMF C26 H19 F6 N5 O2



CM 2

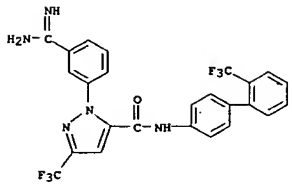
CRN 76-05-1
CMF C2 H F3 O2

RN 209955-27-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-95-0
CMF C25 H17 F6 N5 O

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



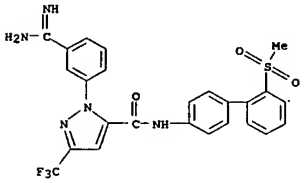
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-28-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-94-9
CMF C25 H20 F3 N5 O3 S



L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

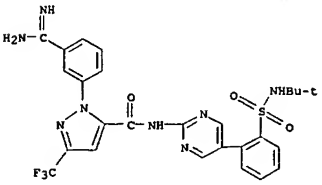
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-37-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-[[(1,1-dimethylethyl)amino]sulfonyl]phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-36-2
CMF C26 H25 F3 N8 O3 S



CM 2

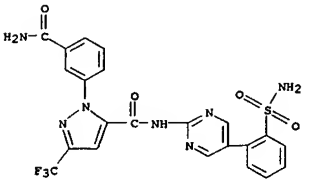
CRN 76-05-1
CMF C2 H F3 O2

RN 209955-41-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, trifluoroacetate (2:1) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

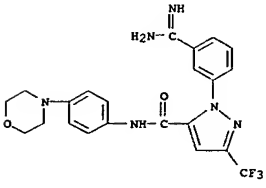
CRN 209955-40-8
CMF C22 H16 F3 N7 O4 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-44-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

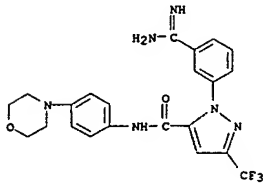


RN 209955-45-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, tris(trifluoroacetate) (9CI)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(CA INDEX NAME)

CM 1

CRN 209955-44-2
CMF C22 H21 F3 N6 O2

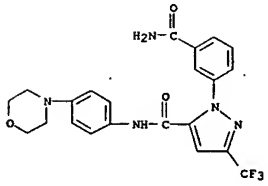


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-46-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

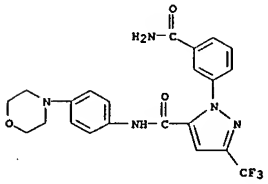
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209955-47-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-46-4
CMF C22 H20 F3 N5 O3

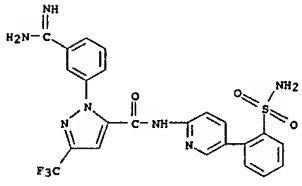


CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

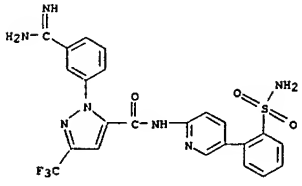
RN 209955-48-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-49-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-48-6
CMF C23 H18 F3 N7 O3 S

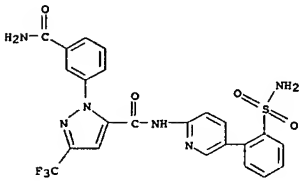


CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

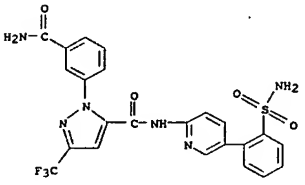
RN 209955-50-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-51-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-50-0
CMF C23 H17 F3 N6 O4 S

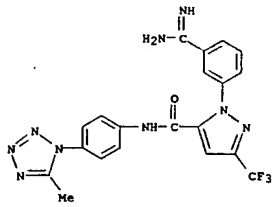


CM 2

CRN 76-05-1

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C2 H F3 O2

RN 209955-52-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-methyl-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-53-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-methyl-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

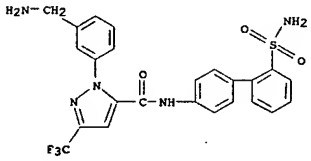
CM 1

CRN 209955-52-2
CMF C20 H16 F3 N9 O

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

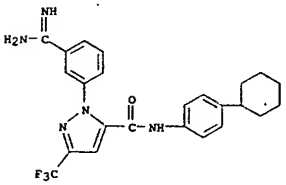
CRN 209955-60-2
CMF C24 H20 F3 N5 O3 S



CM 2

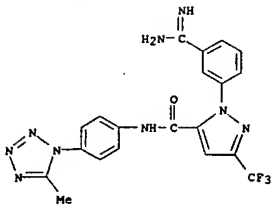
CRN 76-05-1
CMF C2 H F3 O2

RN 209956-54-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-(4-cyclohexylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209956-70-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminoiminomethyl)phenyl]-N-[3-chloro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

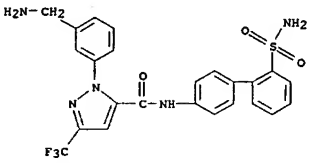
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

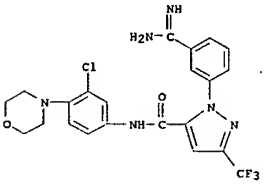
CRN 76-05-1
CMF C2 H F3 O2

RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

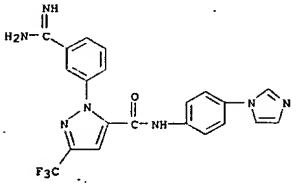


RN 209955-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209956-75-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

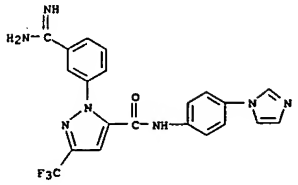


RN 209956-76-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-75-2
CMF C21 H16 F3 N7 O

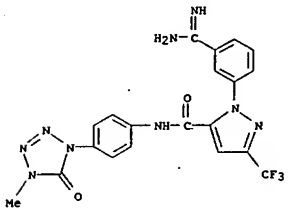
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209956-77-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

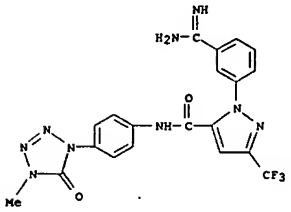


RN 209956-78-5 CAPLUS

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-77-4
CMF C20 H16 F3 N9 O2

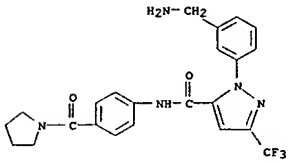


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209956-99-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

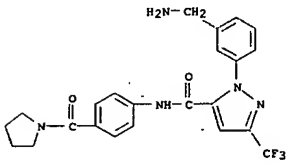
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-00-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-99-0
CMF C23 H22 F3 N5 O2

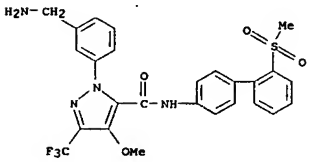


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-27-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

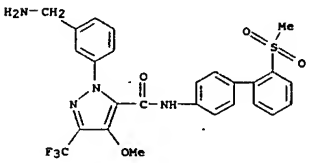
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-28-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-27-7
CMF C26 H23 F3 N4 O4 S

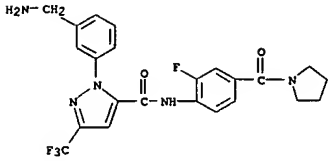


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-29-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

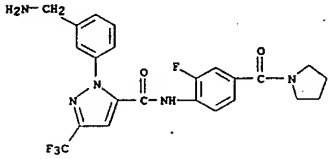
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-30-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-29-9
CMF C23 H21 F4 N5 O2

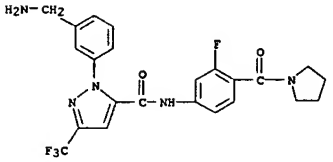


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-31-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

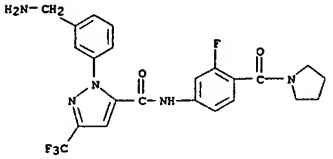
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-32-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-31-3
CMF C23 H21 F4 N5 O2

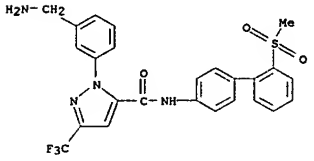


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-33-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

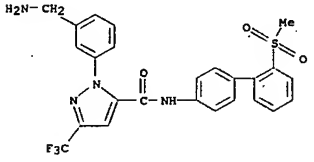
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-34-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-33-5
CMF C25 H21 F3 N4 O3 S

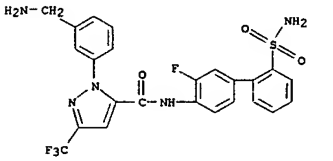


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

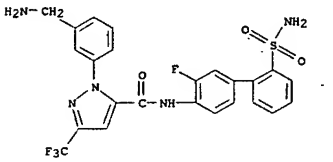
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-36-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-35-7
CMF C24 H19 F4 N5 O3 S



CM 2

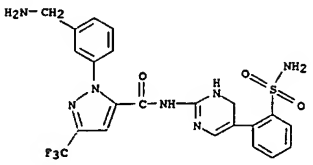
CRN 76-05-1
CMF C2 H F3 O2

RN 209957-38-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209957-37-9
CMF C22 H20 F3 N7 O3 S



CM 2

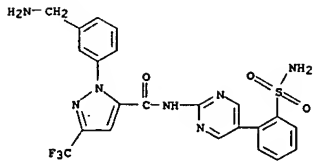
CRN 76-05-1
CMF C2 H F3 O2

RN 209957-40-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-39-1
CMF C22 H18 F3 N7 O3 S

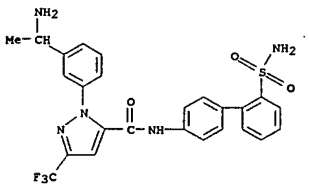
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-41-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(1-aminoethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

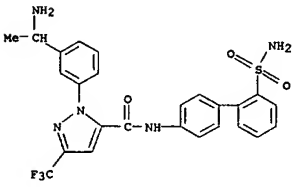


RN 209957-42-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(1-aminoethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

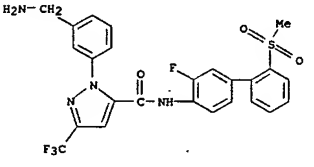
CRN 209957-41-5
CMF C25 H22 F3 N5 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

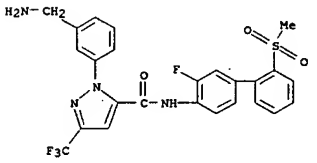


RN 209957-48-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209957-47-1
CMF C25 H20 F4 N4 O3 S



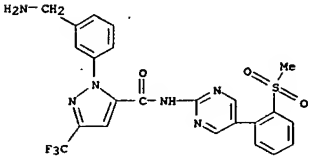
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-50-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-49-3
CMF C23 H19 F3 N6 O3 S

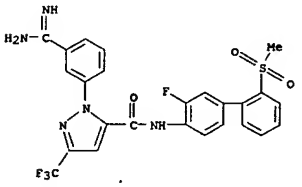


CM 2

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-51-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-52-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

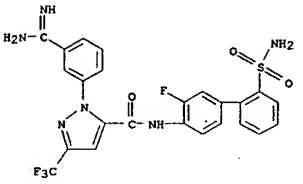
CM 1

CRN 209957-51-7
CMF C25 H19 F4 N5 O3 S

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

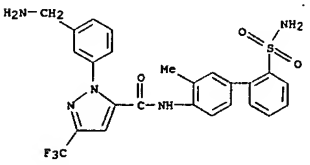
CRN 209957-53-9
CMF C24 H18 F4 N6 O3 S



CM 2

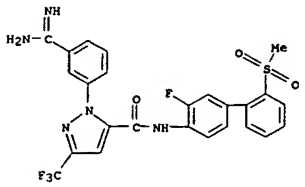
CRN 76-05-1
CMF C2 H F3 O2

RN 209957-67-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-68-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,

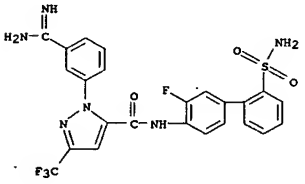
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-53-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

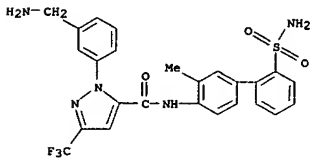


RN 209957-54-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)

CM 1

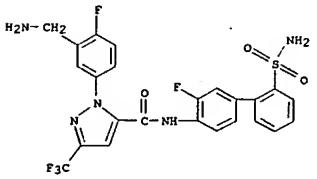
CRN 209957-67-5
CMF C25 H22 F3 N5 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-73-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

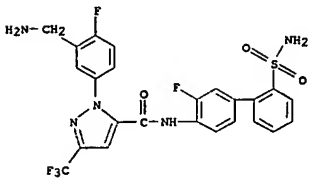


RN 209957-74-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

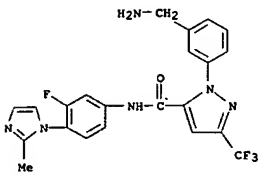
CRN 209957-73-3
CMF C24 H18 F5 N5 O3 S



CM 2

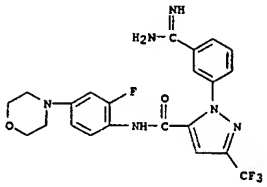
CRN 76-05-1
CMF C2 H F3 O2

RN 209957-83-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

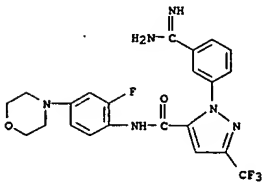
RN 209957-89-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-90-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-89-1
CMF C22 H20 F4 N6 O2

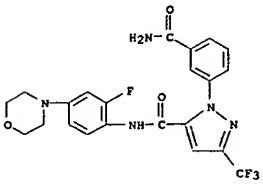


CM 2

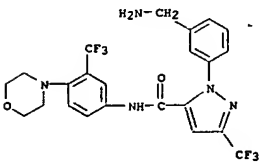
CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209957-91-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-92-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

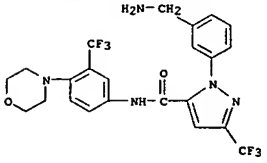


RN 209957-93-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-92-6
CMF C23 H21 F6 N5 O2

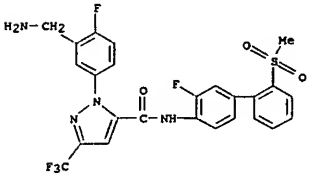
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209958-13-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

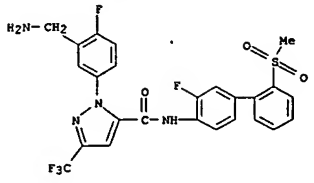


RN 209958-14-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-13-4
CMF C25 H19 F5 N4 O3 S

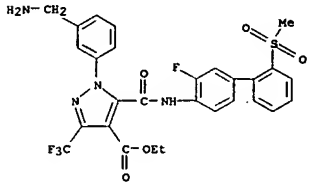
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

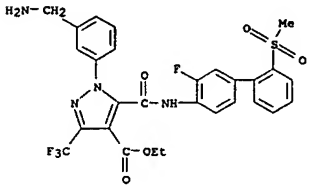
RN 209958-21-4 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 209958-22-5 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-21-4
CMF C28 H24 F4 N4 O5 S

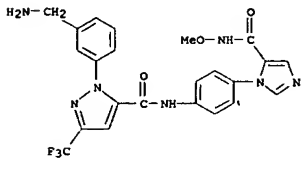


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209958-28-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

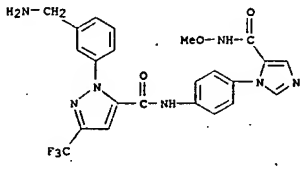
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209958-29-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-28-1
CMF C23 H20 F3 N7 O3

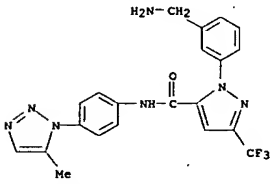


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209958-30-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

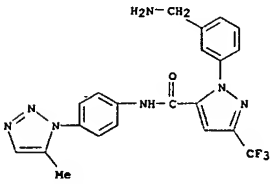
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209958-31-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-30-5
CMF C21 H18 F3 N7 O

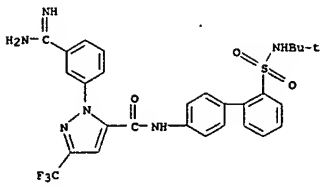


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209958-33-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-

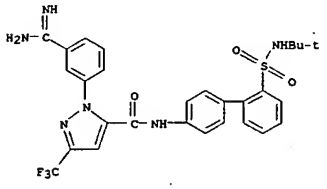
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



RN 256512-05-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, trifluoroacetate (5:6) (9CI) (CA INDEX NAME)

CM 1

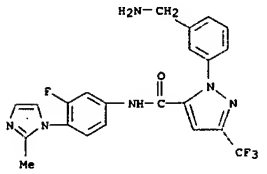
CRN 209958-33-8
CMF C28 H27 F3 N6 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

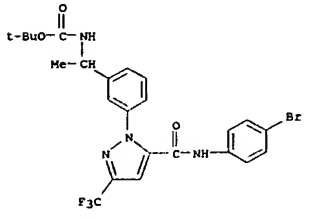
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 209957-83-5
CMF C22 H18 F4 N6 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 209960-02-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azoles as Factor Xa inhibitors)
RN 209960-02-1 CAPLUS
CN Carbamic acid, [1-[3-[5-[[(4-bromophenyl)amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

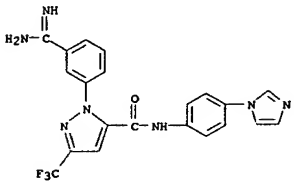


L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 256512-19-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-75-2
CMF C21 H16 F3 N7 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 256512-30-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

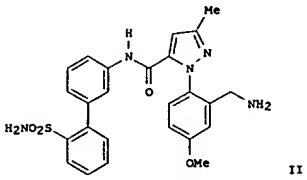
ACCESSION NUMBER: 1999:421659 CAPLUS
DOCUMENT NUMBER: 131:58820
TITLE: Preparation of nitrogen heteroaromatics as blood coagulation factor Xa inhibitors
INVENTOR(S): Galemmo, Robert A., Jr.; Pinto, Donald J. P.; Bostrom, Lori L.; Rossi, Karen Anita
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 237 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9932454 | A1 | 19990701 | WO 1998-US26427 | 19981211 |
| W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| CA 2314401 | A1 | 19990701 | CA 1998-2314401 | 19981211 |
| AU 9917244 | A | 19990712 | AU 1999-17244 | 19981211 |
| BR 9813835 | A | 20001010 | BR 1998-13835 | 19981211 |
| EP 1042299 | A1 | 20001011 | EP 1998-962082 | 19981211 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 2001526268 | T | 20011218 | JP 2000-525391 | 19981211 |
| ZA 9811517 | A | 20000615 | ZA 1998-11517 | 19981215 |
| US 6271237 | B1 | 20010807 | US 1998-217336 | 19981221 |
| US 2002016326 | A1 | 20020207 | US 2001-833302 | 20010412 |
| US 6548525 | B2 | 20030415 | | |

| PRIORITY APPLN. INFO.: | | |
|---|---|---|
| US 1997-68491P | P | 19971222 |
| US 1997-996447 | A | 19971222 |
| US 1998-101075P | P | 19980918 |
| WO 1998-US26427 | W | 19981211 |
| US 1998-217336 | A3 | 19981221 |

OTHER SOURCE(S): MARPAT 131:58820
GI

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



II

AB DEG(CH2)sMZAB [I; D = cyano, amino(alkyl), amidino, etc.; E = (un)substituted phenylene, -pyridinediyl, -pyrimidinediyl, etc.; G = bond, NHCH2, OCH2, SCH2; M = (un)substituted pyrrolylene, -di-, -tri-, or -tetrazolylene; Z = (heteroatom-interrupted)(oxo)alkylene, oxyalkylene, alkyleneoxy, etc.; A = (un)substituted carbocyclic residue (sic) or -heterocyclylene; B = amino(alkyl), amidino, ureido, (un)substituted carbocyclic residue, etc.; s = 0-2] were prepared Thus, 2-hydrazino-5-methoxybenzoic acid was cyclocondensed with MeCOCH2C(:NOMe)CO2Et (preparation each given) and the product converted in 3 steps to 3-methyl-1-(2-azidomethyl-4-methoxyphenyl)-1H-pyrazole-5-carboxylic acid which was amidated by 4-(H2N)C6H4C6H4(CO2NHCMe3)-2 to give, in 2 addnl. steps, title compound II. Data for biol. activity of I were given.

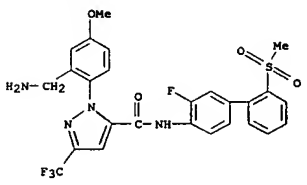
IT 228258-60-4P 228258-88-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of nitrogen heteroaroms. as blood coagulation factor Xa inhibitors)

RN 228258-60-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-56-5
CMF C26 H22 F4 N4 O4 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



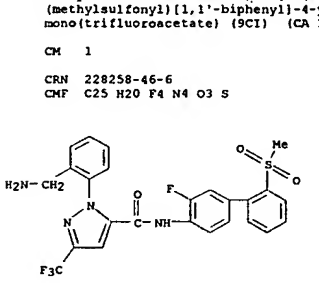
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-88-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-46-6
CMF C25 H20 F4 N4 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 228257-38-3P 228257-41-8P 228257-44-1P
228257-47-4P 228257-50-9P 228257-53-2P
228257-56-5P 228257-59-8P 228257-62-3P
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228257-74-7P 228257-77-0P 228257-80-5P
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228257-92-9P 228257-95-2P 228257-98-5P
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228258-10-4P 228258-13-7P 228258-16-0P
228258-19-3P 228258-22-8P 228258-23-9P
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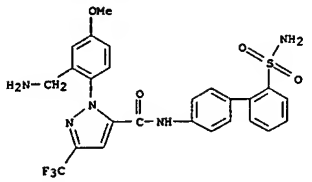
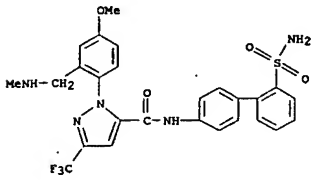
228258-67-1P 228258-68-2P 228258-69-3P
228258-70-6P 228258-71-7P 228258-72-8P
228258-73-9P 228258-74-0P 228258-75-1P
228258-76-2P 228258-77-3P 228258-78-4P
228258-79-5P 228258-80-8P 228258-81-9P
228258-82-0P 228258-83-1P 228258-84-2P
228258-85-3P 228258-86-4P 228258-87-5P
228258-89-7P 228258-90-0P 228258-99-9P
228259-01-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen heteroaroms. as blood coagulation factor Xa inhibitors)

RN 228257-38-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

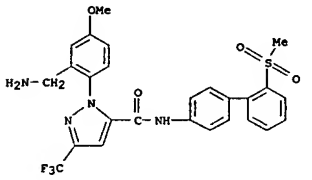
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



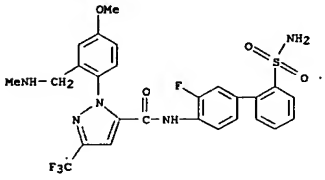
RN 228257-41-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



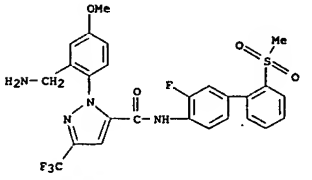
RN 228257-44-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



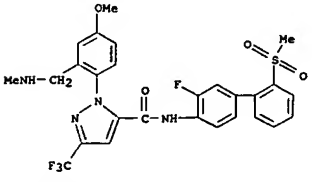
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228257-56-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



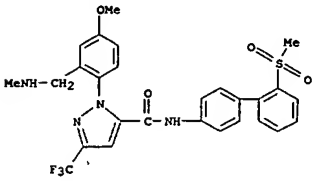
RN 228257-59-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



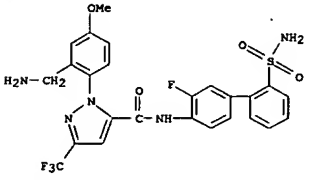
RN 228257-62-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[4-(1-

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 228257-47-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

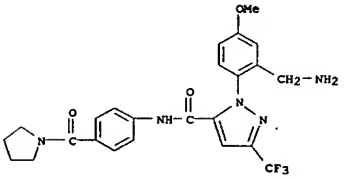


RN 228257-50-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

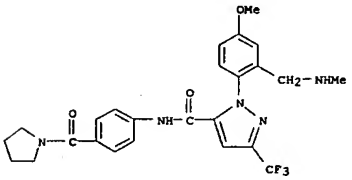


RN 228257-53-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

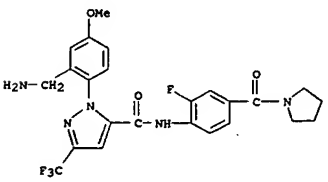
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228257-65-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

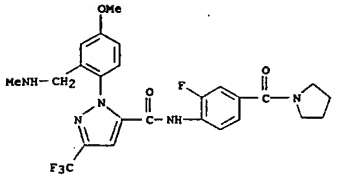


RN 228257-68-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

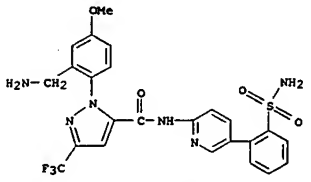


L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 228257-71-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

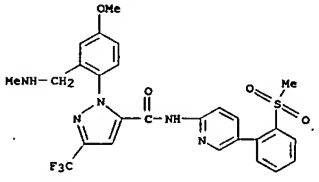


RN 228257-74-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

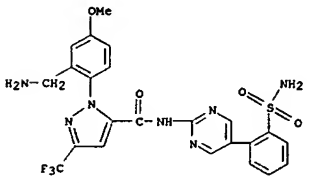


RN 228257-77-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

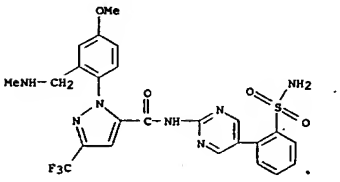
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228257-86-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

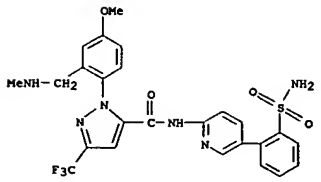


RN 228257-89-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

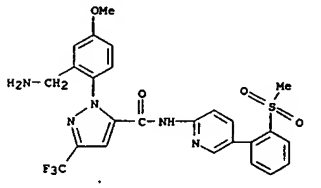


RN 228257-92-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

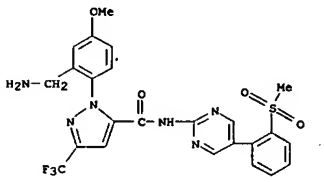


RN 228257-80-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

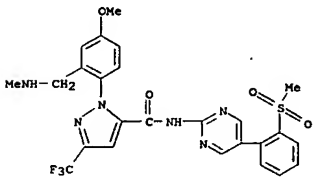


RN 228257-83-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

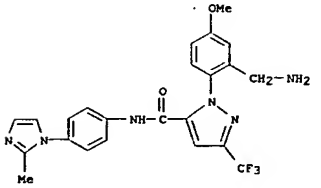
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
INDEX NAME)



RN 228257-95-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

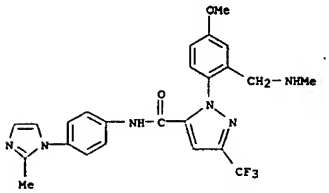


RN 228257-98-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

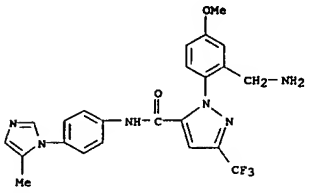


RN 228258-01-3 CAPLUS

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-[4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

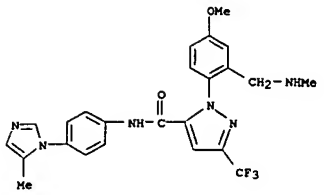


RN 228258-04-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[4-(5-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

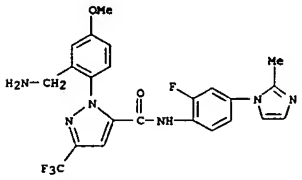


RN 228258-07-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-[4-(5-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

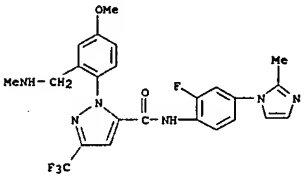


RN 228258-10-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

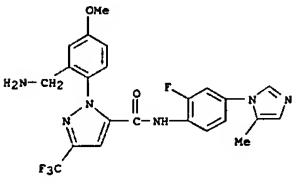


RN 228258-13-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

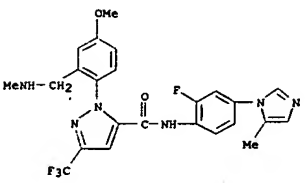
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-16-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2-fluoro-4-(5-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

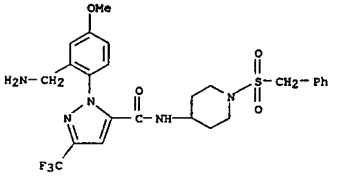


RN 228258-19-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(5-methyl-1H-imidazol-1-yl)phenyl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

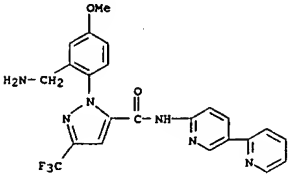


RN 228258-22-8 CAPLUS

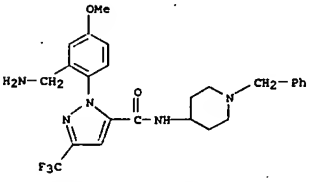
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-[(phenylmethyl)sulfonyl]-4-piperidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-23-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2,3'-bipyridin]-6'-yl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

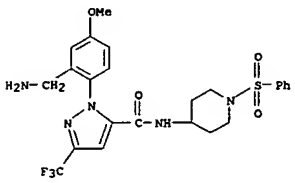


RN 228258-24-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-(phenylmethyl)-4-piperidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

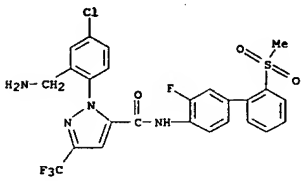


RN 228258-25-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(phenylsulfonyl)-4-piperidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

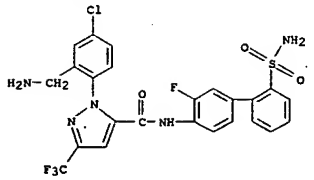


RN 228258-26-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)-4-chlorophenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

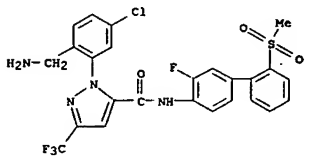


RN 228258-27-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-chlorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

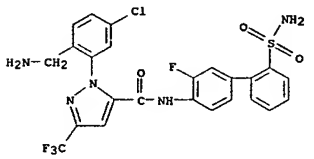
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-28-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)-5-chlorophenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

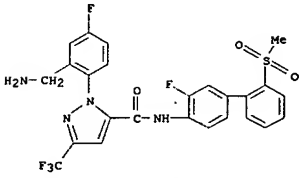


RN 228258-29-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-chlorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

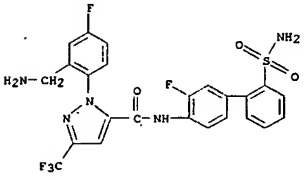


RN 228258-30-8 CAPLUS

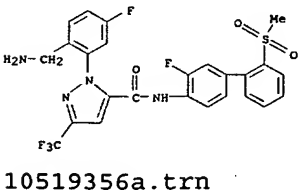
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-31-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

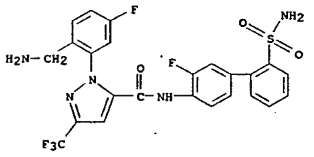


RN 228258-32-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)-5-fluorophenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

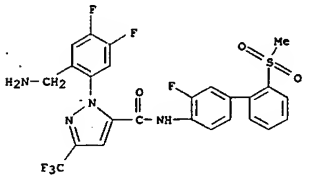


L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 228258-33-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

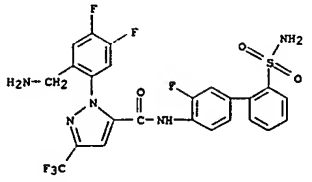


RN 228258-34-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4,5-difluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI)
(CA INDEX NAME)

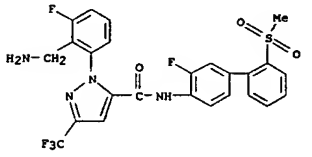


RN 228258-35-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4,5-difluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

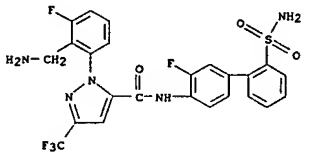
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-36-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-3-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

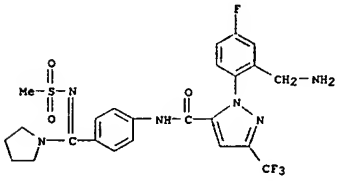


RN 228258-37-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-3-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

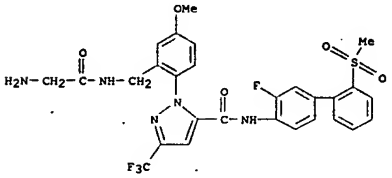


RN 228258-38-6 CAPLUS

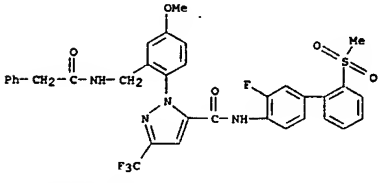
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-41-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[(aminoacetyl)amino]methyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

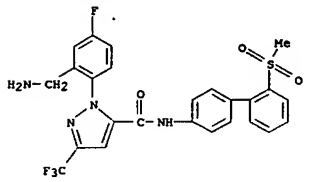


RN 228258-42-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[(phenylacetyl)amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

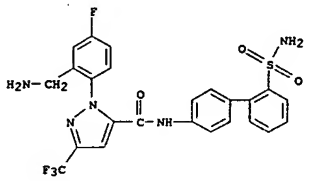


RN 228258-43-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

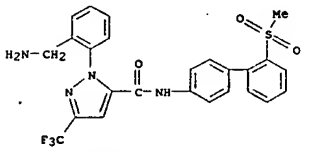


RN 228258-39-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

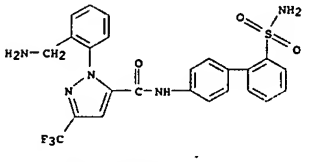


RN 228258-40-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[4-[[(methylsulfonyl)imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

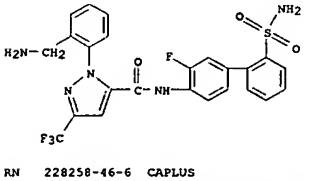
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-44-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

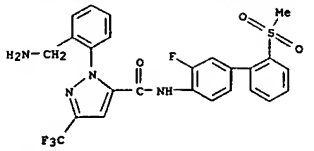


RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

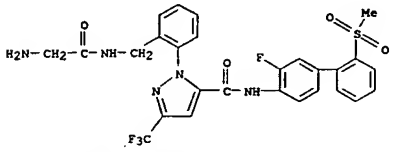


RN 228258-46-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

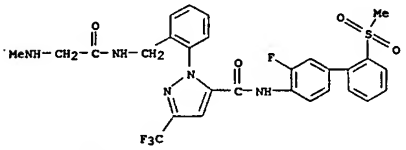
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-47-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[(aminoacetyl)amino]methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

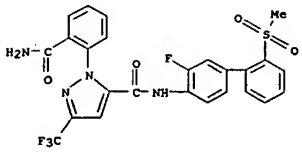


RN 228258-48-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-[[[(methylamino)acetyl]amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-49-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminocarbonyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

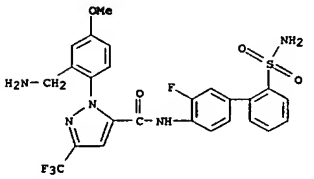
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-59-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-50-9
CMF C25 H21 F4 N5 O4 S



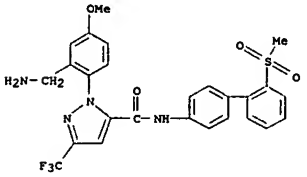
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-61-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-44-1
CMF C26 H23 F3 N4 O4 S



CM 2

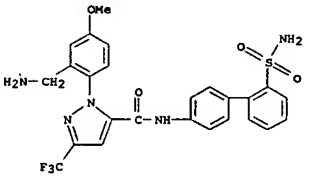
CRN 76-05-1
CMF C2 H F3 O2

RN 228258-62-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-38-3
CMF C25 H22 F3 N5 O4 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



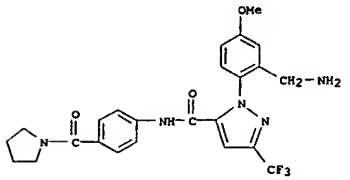
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-63-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-62-3
CMF C24 H24 F3 N5 O3



CM 2

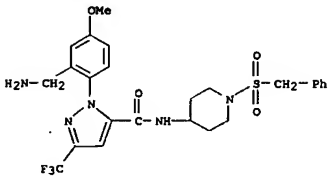
CRN 76-05-1

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C2 H F3 O2

RN 228258-64-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-[(phenylmethyl)sulfonyl]-4-piperidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-22-8
CMF C25 H28 F3 N5 O4 S



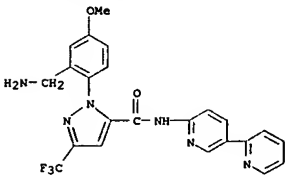
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-65-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



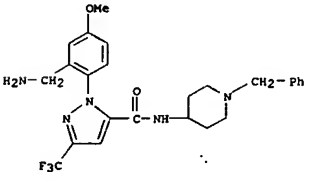
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-67-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-(phenylmethyl)-4-piperidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-24-0
CMF C25 H28 F3 N5 O2



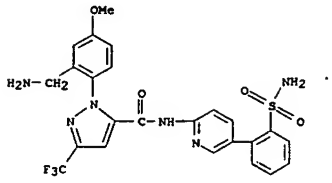
CM 2

CRN 76-05-1



L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 228257-74-7
CMF C24 H21 F3 N6 O4 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-66-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2,3'-bipyridin]-6'-yl-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

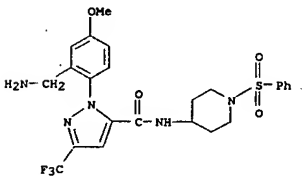
CRN 228258-23-9
CMF C23 H19 F3 N6 O2

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C2 H F3 O2

RN 228258-68-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-(phenylsulfonyl)-4-piperidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-25-1
CMF C24 H26 F3 N5 O4 S



CM 2

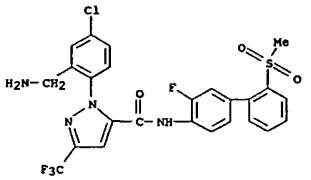
CRN 76-05-1
CMF C2 H F3 O2

RN 228258-69-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-chlorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-26-2
CMF C25 H19 Cl F4 N4 O3 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



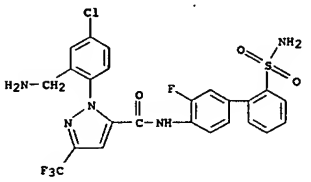
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-70-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-chlorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

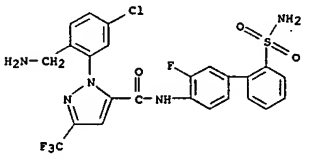
CRN 228258-27-3
CMF C24 H18 Cl F4 N5 O3 S



L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-29-5
CMF C24 H18 Cl F4 N5 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-73-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-30-8
CMF C25 H19 F5 N4 O3 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

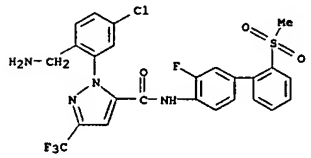
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-71-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-chlorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-28-4
CMF C25 H19 Cl F4 N4 O3 S

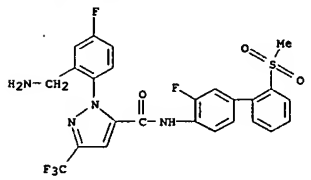


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-72-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-chlorophenyl]-N-[2'-

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



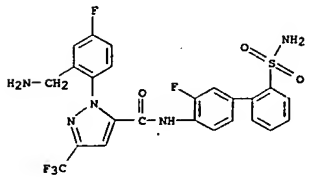
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-74-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-31-9
CMF C24 H18 F5 N5 O3 S



CM 2

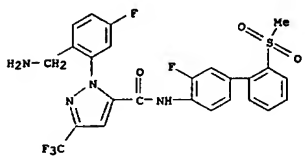
CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 228258-75-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-32-0
CMF C25 H19 F5 N4 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-76-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

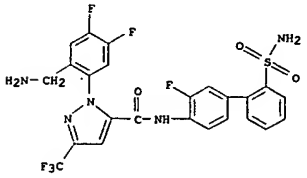
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-78-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4,5-difluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-35-3
CMF C24 H17 F6 N5 O3 S



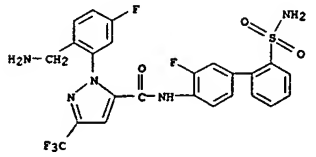
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-79-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-3-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 228258-33-1
CMF C24 H18 F5 N5 O3 S



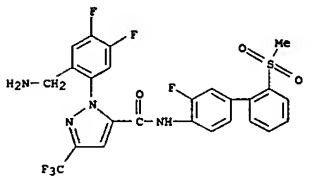
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-77-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4,5-difluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

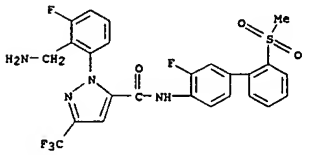
CRN 228258-34-2
CMF C25 H18 F6 N4 O3 S



L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 228258-36-4
CMF C25 H19 F5 N4 O3 S



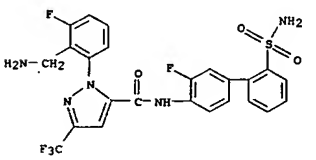
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-80-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-3-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-37-5
CMF C24 H18 F5 N5 O3 S



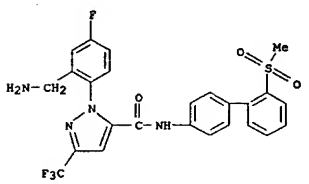
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-81-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-38-6
CMF C25 H20 F4 N4 O3 S

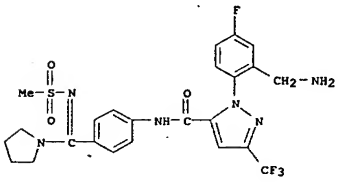


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-82-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



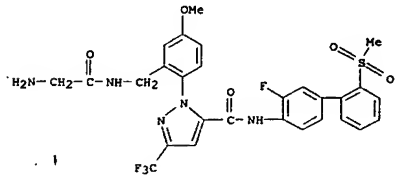
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-84-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[(aminoacetyl)amino]methyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-41-1
CMF C28 H25 F4 N5 O5 S



CM 2

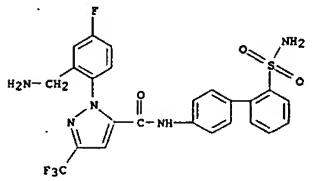
CRN 76-05-1



L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-39-7
CMF C24 H19 F4 N5 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-83-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[4-[[(methylsulfonyl)imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

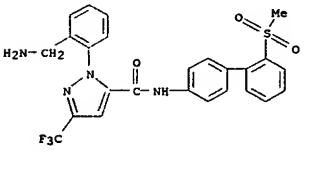
CRN 228258-40-0
CMF C24 H24 F4 N6 O3 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C2 H F3 O2

RN 228258-85-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-43-3
CMF C25 H21 F3 N4 O3 S



CM 2

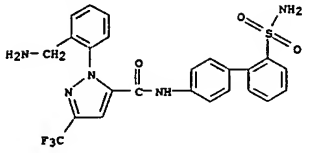
CRN 76-05-1
CMF C2 H F3 O2

RN 228258-86-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-44-4
CMF C24 H20 F3 N5 O3 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



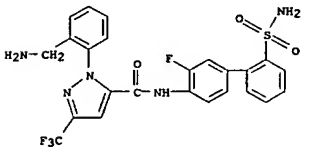
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-87-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-(2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-45-5
CMF C24 H19 F4 N5 O3 S

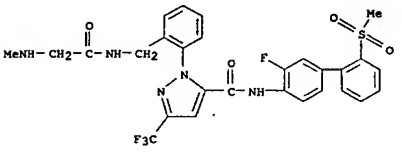


CM 2

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 228258-48-8
CMF C28 H25 F4 N5 O4 S



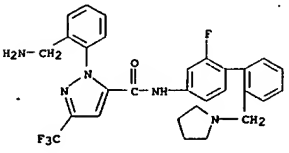
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-99-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-fluoro-2'-(1-pyrrolidinylmethyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-98-8
CMF C29 H27 F4 N5 O



CM 2

CRN 76-05-1

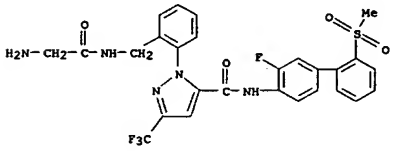
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-89-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[(aminoacetyl)amino]methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-47-7
CMF C27 H23 F4 N5 O4 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 228258-90-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-[[[(methylamino)acetyl]amino]methyl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

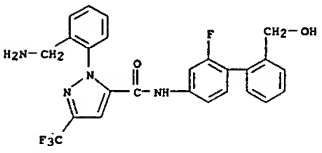
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CMF C2 H F3 O2

RN 228259-01-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-fluoro-2'-(hydroxymethyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 228259-00-5
CMF C25 H20 F4 N4 O2



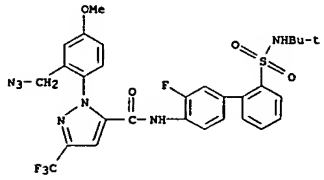
CM 2

CRN 76-05-1
CMF C2 H F3 O2

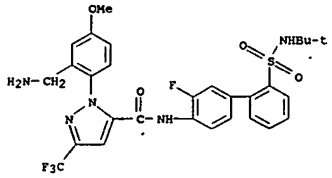
IT 228259-20-9P 228259-21-0P 228259-22-1P
228259-23-2P 228259-24-3P 228259-25-4P
228259-29-8P 228259-36-7P 228259-37-8P
228259-38-9P 228259-39-0P 228259-68-5P
228259-69-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen heteroaroms. as blood coagulation factor Xa inhibitors)

RN 228259-20-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(trifluoromethyl)- (9CI) (CA INDEX NAME)

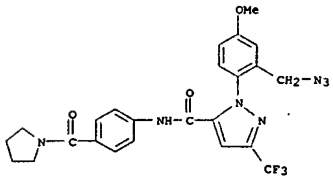


RN 228259-21-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

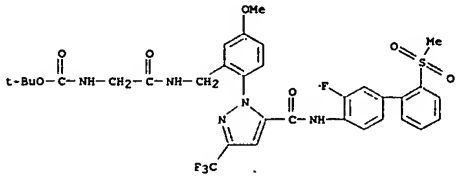


RN 228259-22-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(azidomethyl)-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

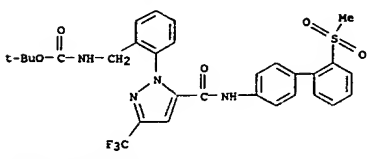
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 228259-25-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



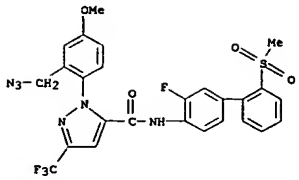
RN 228259-29-8 CAPLUS
CN Carbamic acid,
[2-[[[2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]-5-methoxyphenyl]methyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



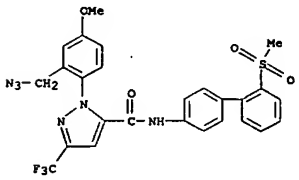
RN 228259-36-7 CAPLUS
CN Carbamic acid, [[2-[5-[[[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



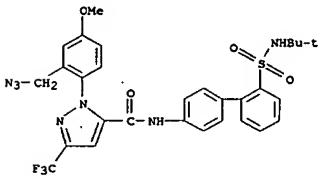
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228259-23-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

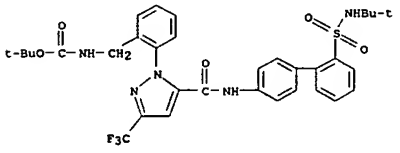


RN 228259-24-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

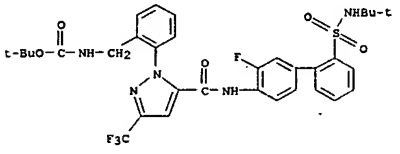


L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

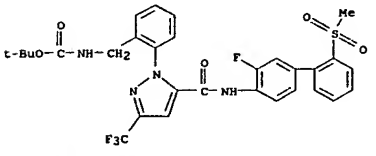
RN 228259-37-8 CAPLUS
CN Carbamic acid, [[2-[5-[[[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 228259-38-9 CAPLUS
CN Carbamic acid, [[2-[5-[[[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

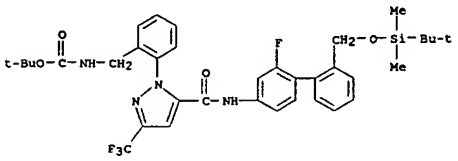


RN 228259-39-0 CAPLUS
CN Carbamic acid, [[2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

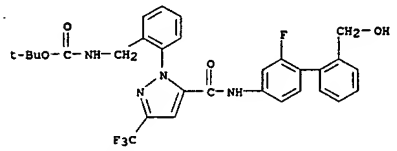


RN 228259-68-5 CAPLUS
CN Carbamic acid,
[[2-[5-[[[2'-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
]-2-fluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl}-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 228259-69-6 CAPLUS
CN Carbamic acid, [[2-[5-[[[2-fluoro-2'-(hydroxymethyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

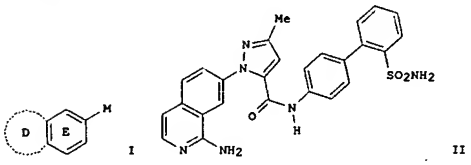
L9 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:9833 CAPLUS
DOCUMENT NUMBER: 130:66494
TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John Matthew; Han, Qi; Li, Renhua; Pinto, Donald Joseph-Phillip; Pruitt, James Russell; Quan, Mimi Lifen
PATENT ASSIGNEE(S): The Du Pont Merck Pharmaceutical Company, USA
SOURCE: PCT Int. Appl., 268 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9857951 | A1 | 19981223 | WO 1998-US12680 | 19980618 |
| W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| ZA 9805247 | A | 19991217 | ZA 1998-5247 | 19980617 |
| CA 2291442 | A1 | 19981223 | CA 1998-2291442 | 19980618 |
| AU 9879768 | A | 19990104 | AU 1998-79768 | 19980618 |
| AU 756755 | B2 | 20030123 | | |
| EP 991638 | A1 | 20000412 | EP 1998-930361 | 19980618 |
| EP 991638 | B1 | 20050817 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO | | | | |
| BR 9810137 | A | 20000808 | BR 1998-10137 | 19980618 |
| EE 9900583 | A | 20000815 | EE 1999-583 | 19980618 |
| EE 4153 | B1 | 20031015 | | |
| HU 200002686 | A2 | 20020128 | HU 2000-2686 | 19980618 |
| JP 2002505686 | T | 20020219 | JP 1999-504785 | 19980618 |
| NZ 502370 | A | 20021025 | NZ 1998-502370 | 19980618 |
| AT 302198 | T | 20050915 | AT 1998-930361 | 19980618 |
| ES 2244064 | T3 | 20051201 | ES 1998-930361 | 19980618 |
| RO 120543 | B1 | 20060330 | RO 1999-1317 | 19980618 |
| TW 544453 | B | 20030801 | TW 1998-87109910 | 19980819 |
| NO 9905965 | A | 19991203 | NO 1999-5965 | 19991203 |
| NO 318359 | B1 | 20050307 | | |
| MX 9911908 | A | 20000531 | MX 1999-11908 | 19991216 |
| LV 12496 | B | 20010120 | LV 1999-178 | 19991216 |
| LT 4705 | B | 20000925 | LT 1999-147 | 19991217 |
| PRIORITY APPLN. INFO.: | | | US 1997-878884 A | 19970619 |
| | | | WO 1998-US12680 W | 19980618 |

OTHER SOURCE(S): MARPAT 130:66494
GI

L9 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



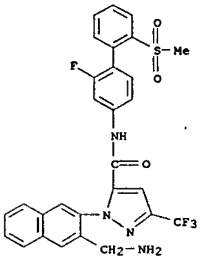
I II

AB The title compds. [I; rings D-E represent guanidine mimics; ring D = CH2N:CH, CH2CH2N:CH, a 5-6 membered aromatic system containing 0-2 heteroatoms selected form the group N, O, and S; ring D is substituted with 0-2 R (substituents), provided that when ring D is unsubstituted, it contains at least one heteroatom; ring E contains 0-2 N atom and is substituted by 0-1 R; R = halo, OH, C1-3 alkoxy, etc.; M = (un)substituted pyrazole, imidazole, tetrazole, etc.], inhibitors of factor Xa which are useful in treating and preventing a thromboembolic disorder, were prepared and formulated. Thus, a multi-step synthesis of the title compound II, starting with 7-aminoisoquinoline, was described. A number of compds. I were found to exhibit a Ki of ≤ 15 μM against factor Xa.

IT 218299-04-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel guanidine mimics as factor Xa inhibitors)

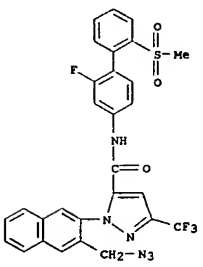
RN 218299-04-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-2-naphthalenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 218302-16-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel guanidine mimics as factor Xa inhibitors)

RN 218302-16-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(azidomethyl)-2-naphthalenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



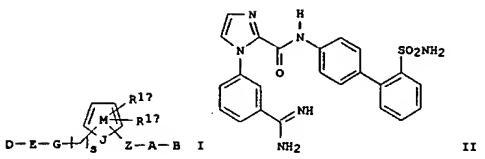
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:479506 CAPLUS
DOCUMENT NUMBER: 129:109090
TITLE: Preparation of nitrogen-containing heteroaromatics as factor Xa inhibitors
INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell; Cacciola, Joseph; Fevig, John Matthew; Han, Qi; Orwat, Michael James; Quan, Mimi Lifen; Rossi, Karen Anita
PATENT ASSIGNEE(S): The Dupont Merck Pharmaceutical Co., USA
SOURCE: PCT Int. Appl., 438 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9828269 | A1 | 19980702 | WO 1997-US22895 | 19971215 |
| W: AM, AU, AZ, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KG, KR, KZ, LT, LV, MD, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, UA, VN | | | | |
| RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| CA 2275796 | A1 | 19980702 | CA 1997-2275796 | 19971215 |
| AU 9856020 | A | 19980717 | AU 1998-56020 | 19971215 |
| AU 730224 | B2 | 20010301 | | |
| EP 946508 | A1 | 19991006 | EP 1997-952409 | 19971215 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI | | | | |
| EE 9900316 | A | 20000215 | EE 1999-316 | 19971215 |
| SI 20017 | A | 20000229 | SI 1997-20082 | 19971215 |
| CN 1246847 | A | 20000308 | CN 1997-181852 | 19971215 |
| BR 9714073 | A | 20000509 | BR 1997-14073 | 19971215 |
| HU 200000735 | A2 | 20010428 | HU 2000-735 | 19971215 |
| JP 2001509145 | T | 20010710 | JP 1998-528845 | 19971215 |
| ZA 9711586 | A | 19990701 | ZA 1997-11586 | 19971223 |
| TW 492971 | B | 20020701 | TW 1997-86119637 | 19980203 |
| NO 9902633 | A | 19990820 | NO 1999-2633 | 19990601 |
| NO 313190 | B1 | 20020826 | | |
| MX 9905878 | A | 20000131 | MX 1999-5878 | 19990622 |
| LT 4673 | B | 20000725 | LT 1999-76 | 19990622 |
| LV 12430 | B | 20000720 | LV 1999-99 | 19990730 |
| PRIORITY APPLN. INFO.: | | | US 1996-769859 A | 19961223 |
| | | | US 1997-879944 A | 19970620 |
| | | | WO 1997-US22895 W | 19971215 |

OTHER SOURCE(S): MARPAT 129:109090
GI




AB The title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(:NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = C1-4 alkylene, (CH2)rO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded the title compound II. A number of compds. I were found to exhibit a Ki of ≤ 10 μM against factor Xa. Some compds. I were evaluated and found to exhibit Ki of < 10 μM against thrombin.

IT 209954-60-9P 209954-61-0P 209954-62-1P
209954-94-9P 209954-95-0P 209954-96-1P
209955-26-0P 209955-27-1P 209955-28-2P
209955-36-2P 209955-37-3P 209955-38-4P
209955-39-5P 209955-40-8P 209955-41-9P
209955-44-2P 209955-45-3P 209955-46-4P
209955-47-5P 209955-48-6P 209955-49-7P
209955-50-0P 209955-51-1P 209955-52-2P
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209956-71-8P 209956-75-2P 209956-76-3P
209956-77-4P 209956-78-5P 209956-99-0P
209957-00-6P 209957-27-7P 209957-28-8P
209957-29-9P 209957-30-2P 209957-31-3P
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209957-35-7P 209957-36-8P 209957-37-9P
209957-38-0P 209957-39-1P 209957-40-4P

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
209957-41-5P 209957-42-6P 209957-47-1P
209957-48-2P 209957-49-3P 209957-50-6P
209957-51-7P 209957-52-8P 209957-53-9P
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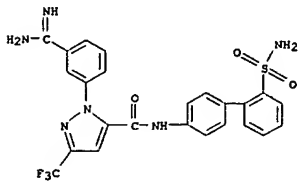
209957-73-3P 209957-74-4P 209957-83-5P
209957-84-6P 209957-89-1P 209957-90-4P
209957-91-5P 209957-92-6P 209957-93-7P
209958-13-4P 209958-14-5P 209958-21-4P
209958-22-5P 209958-28-1P 209958-29-2P
209958-30-5P 209958-31-6P 209958-33-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nitrogen-contg. heteroaroms. as factor Xa inhibitors)

RN 209954-60-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-59-6
CMF C24 H19 F3 N6 O3 S

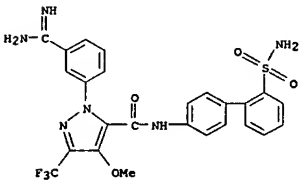


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209954-61-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-4-methoxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

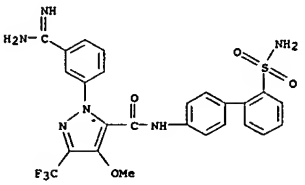
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209954-62-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-4-methoxy-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-61-0
CMF C25 H21 F3 N6 O4 S

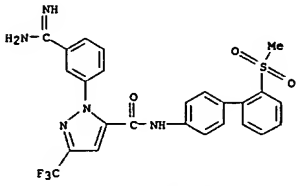


CM 2

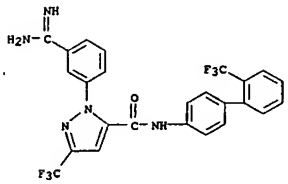
CRN 76-05-1
CMF C2 H F3 O2

RN 209954-94-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

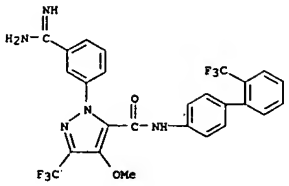


RN 209954-95-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 209954-96-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-4-methoxy-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

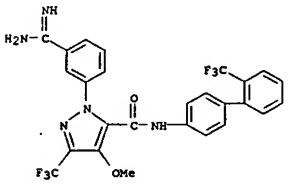
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209955-26-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-4-methoxy-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-96-1
CMF C26 H19 F6 N5 O2



CM 2

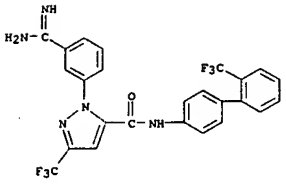
CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209955-27-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-95-0
CMF C25 H17 F6 N5 O



CM 2

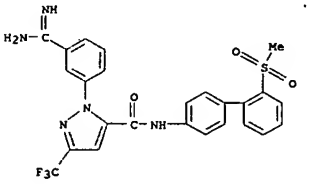
CRN 76-05-1
CMF C2 H F3 O2

RN 209955-28-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-94-9
CMF C25 H20 F3 N5 O3 S

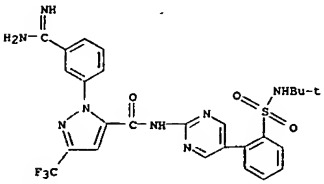
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-36-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-[[(1,1-dimethylethyl)amino]sulfonyl]phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

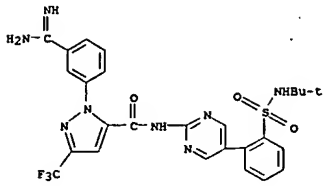


RN 209955-37-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-[[(1,1-dimethylethyl)amino]sulfonyl]phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-36-2

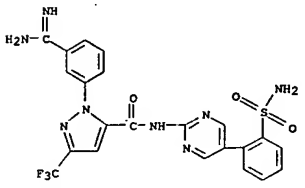
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C26 H25 F3 N8 O3 S



CM 2

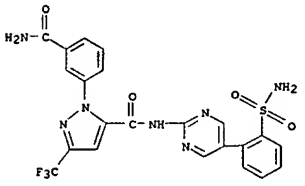
CRN 76-05-1
CMF C2 H F3 O2

RN 209955-38-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-39-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-

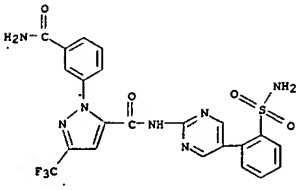
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209955-41-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, trifluoroacetate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-40-8
CMF C22 H16 F3 N7 O4 S



CM 2

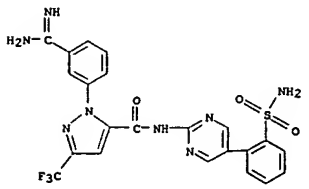
CRN 76-05-1
CMF C2 H F3 O2

RN 209955-44-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-38-4
CMF C22 H17 F3 N8 O3 S

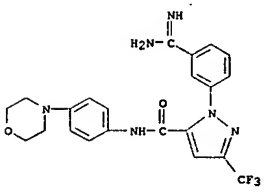


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-40-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

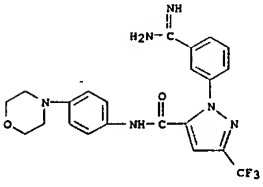
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209955-45-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-44-2
CMF C22 H21 F3 N6 O2

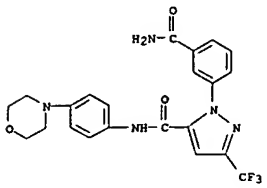


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-46-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(4-

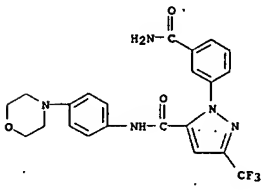
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-47-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

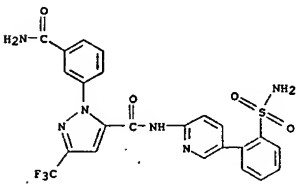
CRN 209955-46-4
CMF C22 H20 F3 N5 O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-50-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-51-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

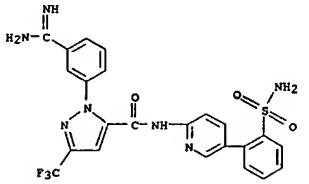
CM 1

CRN 209955-50-0
CMF C23 H17 F3 N6 O4 S



L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

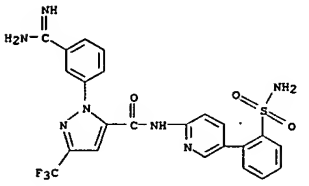
RN 209955-48-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



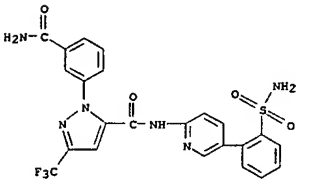
RN 209955-49-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-48-6
CMF C23 H18 F3 N7 O3 S



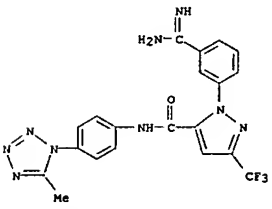
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-52-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-methyl-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

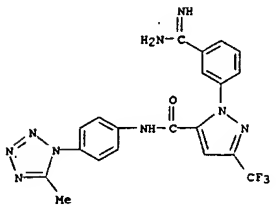


RN 209955-53-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-methyl-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-52-2

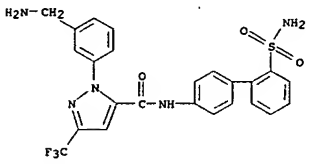
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C20 H16 F3 N9 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



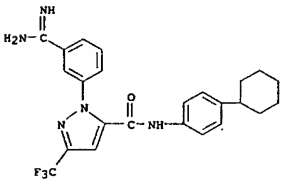
RN 209955-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209956-55-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-(4-cyclohexylphenyl)-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-54-7
CMF C24 H24 F3 N5 O



CM 2

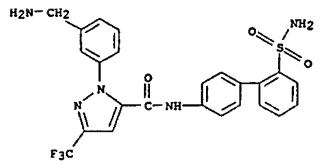
CRN 76-05-1
CMF C2 H F3 O2

RN 209956-70-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-chloro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

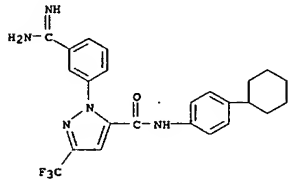
CRN 209955-60-2
CMF C24 H20 F3 N5 O3 S



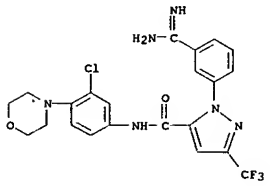
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209956-54-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-(4-cyclohexylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



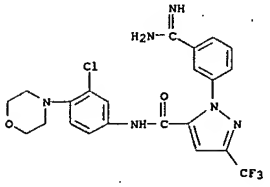
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209956-71-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-chloro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-70-7
CMF C22 H20 Cl F3 N6 O2

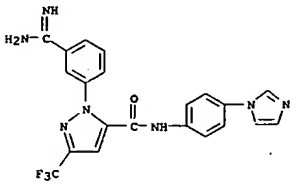


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209956-75-2 CAPLUS

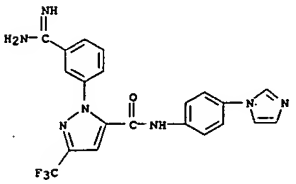
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209956-76-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

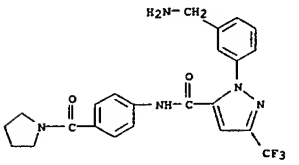
CRN 209956-75-2
CMF C21 H16 F3 N7 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209956-99-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-00-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

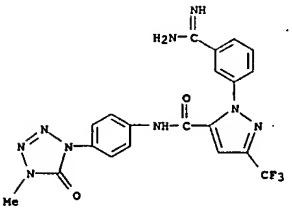
CM 1

CRN 209956-99-0
CMF C23 H22 F3 N5 O2



L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209956-77-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

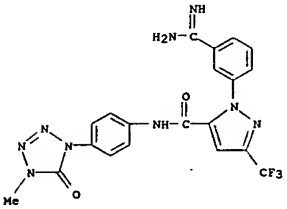


RN 209956-78-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-77-4
CMF C20 H16 F3 N9 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 209957-27-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

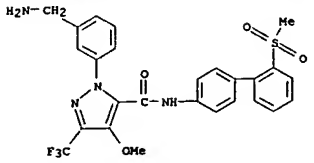


RN 209957-28-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-27-7
CMF C26 H23 F3 N4 O4 S

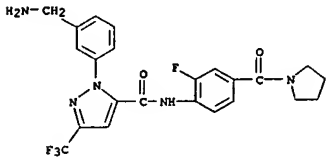
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-29-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

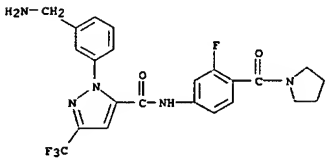


RN 209957-30-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-29-9
CMF C23 H21 F4 N5 O2

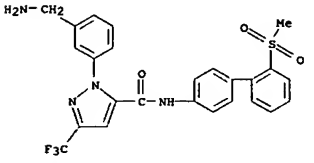
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-33-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

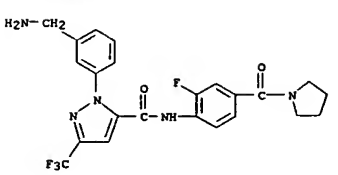


RN 209957-34-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-33-5
CMF C25 H21 F3 N4 O3 S

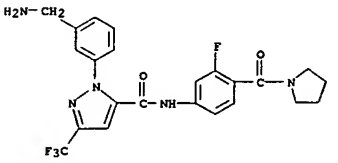
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-31-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

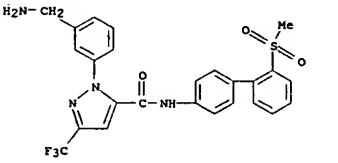


RN 209957-32-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-31-3
CMF C23 H21 F4 N5 O2

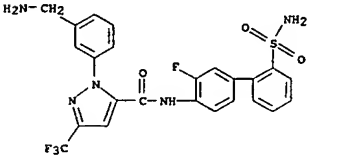
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

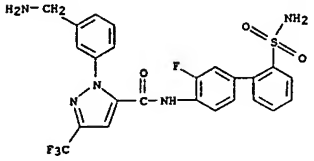


RN 209957-36-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-35-7
CMF C24 H19 F4 N5 O3 S

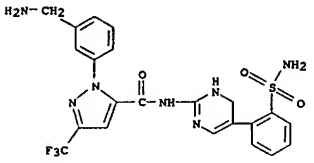
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-37-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)



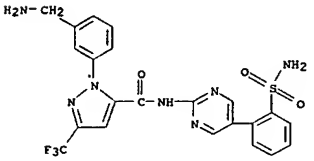
RN 209957-38-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-37-9
CMF C22 H20 F3 N7 O3 S

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

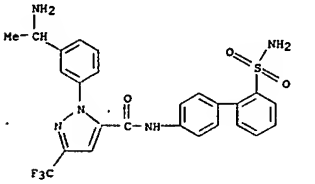
CRN 209957-39-1
CMF C22 H18 F3 N7 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

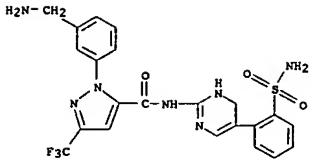
RN 209957-41-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(1-aminoethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-42-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(1-aminoethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

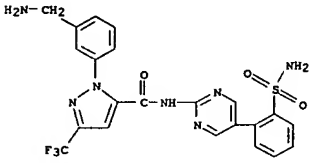
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-39-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

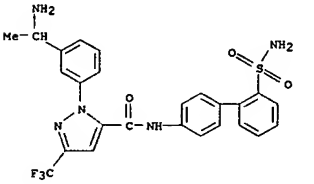


RN 209957-40-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

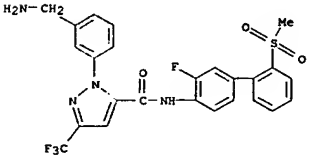
CRN 209957-41-5
CMF C25 H22 F3 N5 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

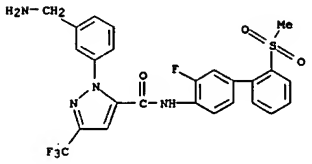


RN 209957-48-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

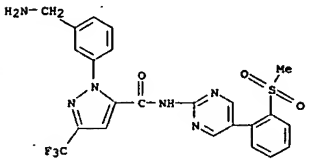
CRN 209957-47-1
CMF C25 H20 F4 N4 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-49-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

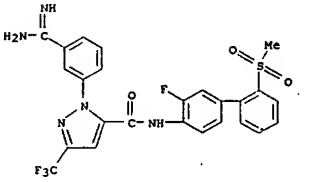


RN 209957-50-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 209957-52-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-51-7
CMF C25 H19 F4 N5 O3 S



CM 2

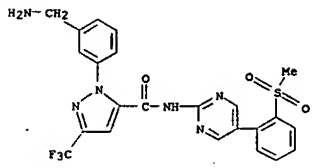
CRN 76-05-1
CMF C2 H F3 O2

RN 209957-53-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

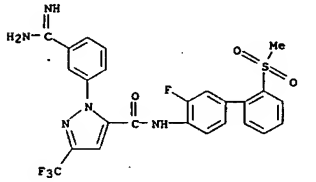
CRN 209957-49-3
CMF C23 H19 F3 N6 O3 S



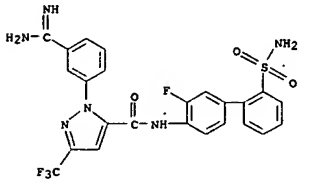
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-51-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



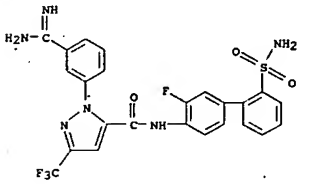
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-54-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-53-9
CMF C24 H18 F4 N6 O3 S

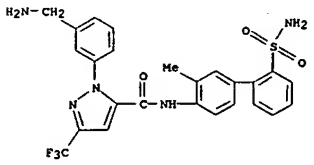


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-67-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-

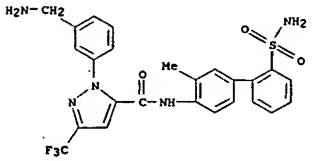
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-68-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-
3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
mono(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM 1

CRN 209957-67-5
CMF C25 H22 F3 N5 O3 S

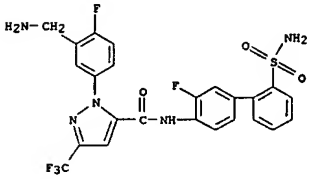


CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

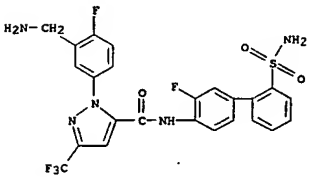
RN 209957-73-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-
(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI)
(CA INDEX NAME)



RN 209957-74-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-
(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-73-3
CMF C24 H18 F5 N5 O3 S

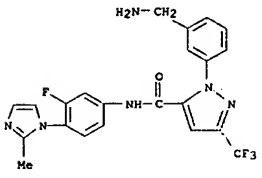


CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

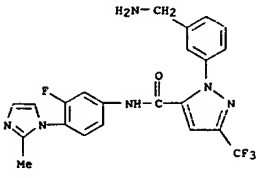
RN 209957-83-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-
methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX
NAME)



RN 209957-84-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-
methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-83-5
CMF C22 H18 F4 N6 O

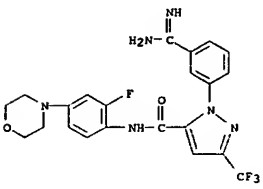


CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

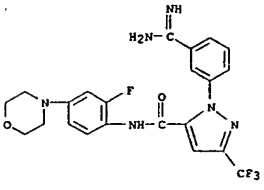
RN 209957-89-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(4-
morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-90-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(4-
morpholinyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI)
(CA
INDEX NAME)

CM 1

CRN 209957-89-1
CMF C22 H20 F4 N6 O2

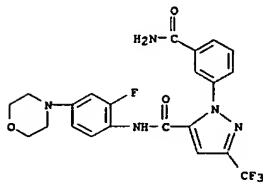


CM 2

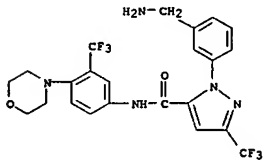
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 76-05-1
CMF C2 H F3 O2

RN 209957-91-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-92-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



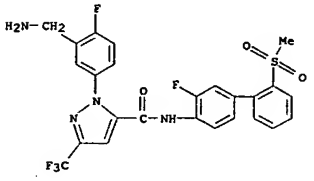
RN 209957-93-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209958-14-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-13-4
CMF C25 H19 F5 N4 O3 S



CM 2

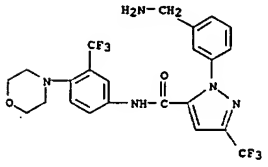
CRN 76-05-1
CMF C2 H F3 O2

RN 209958-21-4 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid,
1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)

CM 1

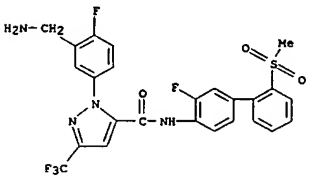
CRN 209957-92-6
CMF C23 H21 F6 N5 O2



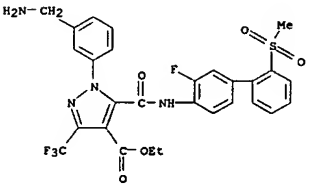
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209958-13-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



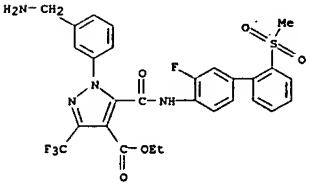
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209958-22-5 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid,
1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-21-4
CMF C28 H24 F4 N4 O5 S

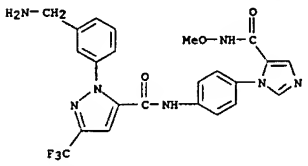


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 209958-28-1 CAPLUS

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-29-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-28-1
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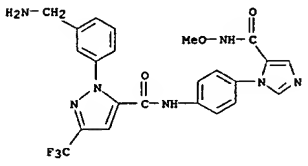
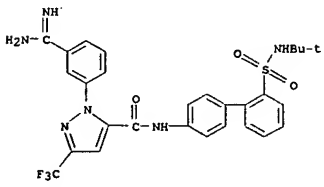


CM 2

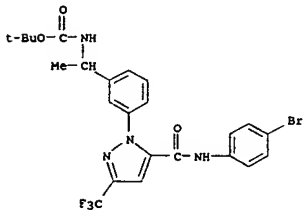
CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209958-33-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT 209960-02-1P 209960-07-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)
RN 209960-02-1 CAPLUS
CN Carbamic acid, [1-[3-[5-[[(4-bromophenyl)amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

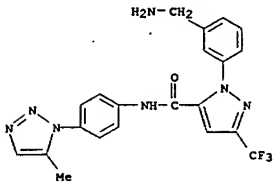


RN 209960-07-6 CAPLUS
CN Carbamic acid, [[3-[5-[[[5-[2-(methylsulfonyl)phenyl]-2-



L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

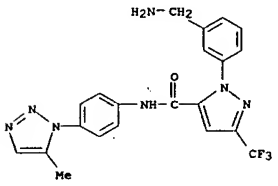
RN 209958-30-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-31-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

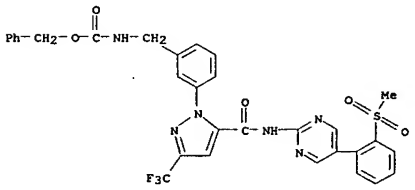
CRN 209958-30-5
CMF C21 H18 F3 N7 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrimidinyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

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FULL ESTIMATED COST                                    199.57     423.85

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -28.08     -35.10

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FULL ESTIMATED COST                                    199.57     423.85

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -28.08     -35.10

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -28.08     -35.10

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FILE LAST UPDATED: 7 Jan 2007 (20070107/ED)

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L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:20490 CAPLUS
DOCUMENT NUMBER: 140:77148
ENTRY DATE: Entered STN: 11 Jan 2004
TITLE: Preparation of N-[4-(thiooxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis
INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsaklakidis, Christos; Gleitz, Johannes; Barnes, Christopher
PATENT ASSIGNEE(S): Merck Patent Gmbh, Germany
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
INT. PATENT CLASSIF.:
MAIN: A61K031-4155
SECONDARY: A61K031-4178; A61K031-433; A61K031-42; C07D403-12; C07D417-12; C07D413-14; C07D403-14
CLASSIFICATION: 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004002477 | A1 | 20040108 | WO 2003-EP5898 | 20030605 |
| WO 2004002477 | A8 | 20040415 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| DE 10229070 | A1 | 20040115 | DE 2002-10229070 | 20020628 |
| CA 2491271 | A1 | 20040108 | CA 2003-2491271 | 20030605 |
| AU 2003238475 | A1 | 20040119 | AU 2003-238475 | 20030605 |
| EP 1517685 | A1 | 20050330 | EP 2003-732540 | 20030605 |
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| JP 2005535630 | T | 20051124 | JP 2004-516575 | 20030605 |
| EP 1679073 | A1 | 20060712 | EP 2006-157 | 20030605 |
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| US 2005203127 | A1 | 20050915 | US 2004-519356 | 20041228 |

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PRIORITY APPLN. INFO.: DE 2002-10229070 A 20020628
EP 2003-732540 A3 20030605

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
WO 2003-EP5898 W 20030605

PATENT CLASSIFICATION CODES:

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
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| WO 2004002477 | ICM | A61K031-4155 |
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| | IPCR | A61K0031-4155 [I,C*]; A61K0031-4155 [I,A]; A61K0031-4164 [I,C*]; A61K0031-4178 [I,A]; A61K0031-42 [I,C*]; A61K0031-42 [I,A]; A61K0031-433 [I,C*]; A61K0031-433 [I,A]; A61P0007-00 [I,C*]; A61P0007-02 [I,A]; A61P0009-00 [I,C*]; A61P0009-08 [I,A]; A61P0009-10 [I,A]; A61P0025-00 [I,C*]; A61P0025-06 [I,A]; A61P0029-00 [I,C*]; A61P0029-00 [I,A]; A61P0035-00 [I,C*]; A61P0035-00 [I,A]; A61P0035-04 [I,A]; A61P0043-00 [I,C*]; A61P0043-00 [I,A]; C07D0403-00 [I,C*]; C07D0403-12 [I,A]; C07D0413-00 [I,C*]; C07D0413-14 [I,A]; C07D0417-00 [I,C*]; C07D0417-12 [I,A] |
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L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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| | | A61K0031-4155 [ICS,7]; A61K0031-4178 [ICS,7]; A61K0031-4164 [ICS,7,C*]; A61K0031-42 [ICS,7]; A61K0031-422 [ICS,7]; A61K0031-433 [ICS,7] |
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| AU 2003238475 | IPCI | A61K0031-4155 [ICM,7]; A61K0031-4178 [ICS,7]; A61K0031-4164 [ICS,7,C*]; A61K0031-433 [ICS,7]; A61K0031-42 [ICS,7]; C07D0403-12 [ICS,7]; C07D0417-12 [ICS,7]; C07D0417-00 [ICS,7,C*]; C07D0413-14 [ICS,7]; C07D0413-00 [ICS,7,C*]; C07D0403-14 [ICS,7]; C07D0403-00 [ICS,7,C*] |
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| EP 1517685 | IPCI | A61K0031-4155 [ICM,7]; A61K0031-4178 [ICS,7]; A61K0031-4164 [ICS,7,C*]; A61K0031-433 [ICS,7]; A61K0031-42 [ICS,7]; C07D0403-12 [ICS,7]; C07D0417-12 [ICS,7]; C07D0417-00 [ICS,7,C*]; C07D0413-14 [ICS,7]; C07D0413-00 [ICS,7,C*]; C07D0403-14 [ICS,7]; C07D0403-00 [ICS,7,C*] |
| | IPCR | A61K0031-4155 [I,C*]; A61K0031-4155 [I,A]; A61K0031-4164 [I,C*]; A61K0031-4178 [I,A]; A61K0031-42 [I,C*]; A61K0031-42 [I,A]; A61K0031-433 [I,C*]; A61K0031-433 [I,A]; A61P0007-00 [I,C*]; A61P0007-02 [I,A]; A61P0009-00 [I,C*]; A61P0009-08 [I,A]; A61P0009-10 [I,A]; A61P0025-00 [I,C*]; A61P0025-06 [I,A]; A61P0029-00 [I,C*]; A61P0029-00 [I,A]; A61P0035-00 [I,C*]; A61P0035-00 [I,A]; A61P0035-04 [I,A]; A61P0043-00 [I,C*]; A61P0043-00 [I,A]; C07D0403-00 [I,C*]; C07D0403-12 [I,A]; C07D0413-00 [I,C*]; C07D0413-14 [I,A]; C07D0417-00 [I,C*]; C07D0417-12 [I,A] |
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L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

| | | |
|---|---|---|
| | | [ICS,7]; C07D0417-00 [ICS,7,C*] |
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| | ECLA | C07D403/12; C07D403/14; C07D413/14; C07D417/12 |
| US 2005203127 | IPCI | C07D0413-02 [ICM,7]; C07D0413-00 [ICM,7,C*]; A61K0031-4709 [ICS,7]; A61K0031-4245 [ICS,7]; A61K0031-423 [ICS,7] |
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| | NCL | 514/310.000; 514/364.000; 514/375.000; 546/146.000; 548/131.000; 548/215.000 |
| | ECLA | A61K031/4155; A61K031/4178; A61K031/42; A61K031/433; C07D403/12+231+207; C07D403/12+233+231; C07D413/14+261+231+207; C07D413/14+261+231+231; C07D417/12+285B+231 |

OTHER SOURCE(S): MARPAT 140:77148
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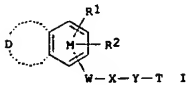


I

ABSTRACT:
Title compds. [I; D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene; H = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(:S)N(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bi)cyclic aromatic (hetero)cyclyl; X = CONR3, CONR3C(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y =

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
alkylene, cycloalkylene, heterodiyl, aryldiyl; T = (substituted) (bi)cyclic arom. heterocyclyl], were prepd. Thus, 333 mg {3-[5-(4-[2-iminopyrrolidin-1-yl]phenylcarbamoyl)-3-trifluoromethylpyrazol-1-yl]benzyl}carbamic acid tert-Bu ester (prepn. given) in EtOH was treated with HCl in ether to give 289 mg N-[4-(2-iminopyrrolidin-1-yl)phenyl]-1-(3-aminomethylphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the receptor Xa with IC50 = 9,6·10-9 M and to the receptor VIIa with IC50 = 2,3·10-8 M.

SUPPL. TERM: iminopyrrolidinylphenylphenylpyrazolecarboxamide prepn coagulation factor Xa inhibitor; phenylpyrazolecarboxamide iminopyrrolidinylphenyl prepn coagulation factor VIIa inhibitor

INDEX TERM: Heart, disease
(angina pectoris, treatment; preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: Brain, disease
(cerebrovascular, treatment; preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: Artery, disease
(coronary, restenosis, treatment; preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: Heart, disease
(infarction, treatment; preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: Artery, disease
(intermittent claudication, treatment; preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: Neoplasm
(metastasis, treatment; preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: Headache
(migraine, treatment; preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
boxamides and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: 612841-24-4P 612841-31-3P 612841-32-4P 612841-34-6P 640287-98-5P 640287-99-6P 640288-00-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S): (1) Du Pont Merck Pharma; WO 9828269 A 1998 CAPLUS
(2) Du Pont Merck Pharma; WO 9857937 A 1998 CAPLUS
(3) Du Pont Merck Pharma; WO 9857951 A 1998 CAPLUS

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

INDEX TERM: Anti-inflammatory agents
Antiarteriosclerotics
Anticoagulants
Antimigraine agents
Antitumor agents
Human
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: Arteriosclerosis
Inflammation
Neoplasm
Thrombosis
(treatment; preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl
derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: 9002-05-5, Coagulation factor Xa 65312-43-8, Coagulation factor VIIa
ROLE: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: 640287-97-4P 640288-03-5P 640288-05-7P 640288-06-8P 640288-07-9P 640288-11-5P 640288-12-6P 640288-13-7P 640288-14-8P 640288-15-9P 640288-16-0P 640288-17-1P 640288-18-2P 640288-19-3P 640288-20-6P 640288-21-7P 640288-22-8P 640288-23-9P 640288-24-0P 640288-25-1P 640288-26-2P 640288-27-3P 640288-28-4P 640288-29-5P 640288-30-8P
ROLE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

INDEX TERM: 209917-93-1 438056-68-9 443999-53-9 625101-83-9 625101-85-1 640288-01-3 640288-02-4 640288-04-6 640288-08-0 640288-09-1 640288-10-4
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)car

=> d hitstr

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

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=> d str
'STR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO.  You may specify the format fields in any order and the
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information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):hitrn

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

=> FIL REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 8.94 | 432.79 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -0.78 | -35.88 |

FILE 'REGISTRY' ENTERED AT 09:08:28 ON 08 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2
DICTIONARY FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> S 640287-97-4/RN

L11 1 640287-97-4/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L11 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):n

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=>

=> d his

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     (FILE 'HOME' ENTERED AT 07:49:52 ON 08 JAN 2007)

     FILE 'REGISTRY' ENTERED AT 07:50:03 ON 08 JAN 2007
L1              STRUCTURE UPLOADED
L2           50 L1

     FILE 'CAPLUS' ENTERED AT 07:50:41 ON 08 JAN 2007
L3           28 L2

     FILE 'REGISTRY' ENTERED AT 07:51:35 ON 08 JAN 2007
L4              STRUCTURE UPLOADED
L5           50 L4
L6              STRUCTURE UPLOADED
L7           22 L6
L8          426 L6 FULL

     FILE 'MEDLINE, CAPLUS' ENTERED AT 07:56:10 ON 08 JAN 2007
L9           36 L8

     FILE 'CAPLUS' ENTERED AT 09:03:48 ON 08 JAN 2007
                E US 2004-519356/AP,PRN 25
L10           1 S E3

     FILE 'REGISTRY' ENTERED AT 09:08:28 ON 08 JAN 2007
L11           1 S 640287-97-4/RN
                SET NOTICE 1 DISPLAY
                SET NOTICE LOGIN DISPLAY

=> d hitstr
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats.  The predefined substance formats
are:  (RN = CAS Registry Number)

REG     - RN
SAM     - Index Name, MF, and structure - no RN
FIDE    - All substance data, except sequence data
IDE     - FIDE, but only 50 names
SQIDE   - IDE, plus sequence data
SQIDE3  - Same as SQIDE, but 3-letter amino acid codes are used
SQD     - Protein sequence data, includes RN
SQD3    - Same as SQD, but 3-letter amino acid codes are used
SQN     - Protein sequence name information, includes RN

CALC    - Table of calculated properties
EPROP   - Table of experimental properties
PROP    - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance.  The substance formats
must be cited first.  The CA File predefined formats are:

ABS  -- Abstract
APPS -- Application and Priority Information
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BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):sam

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI)
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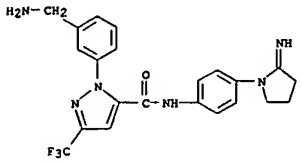

●2 HCl

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640288-16-0P   640288-17-1P
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FIELD CODE - 'AND' OPERATOR ASSUMED '0287-97-4P(W)640288-03-'
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FIELD CODE - 'AND' OPERATOR ASSUMED '0288-05-7P(W)640288-06-'
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FIELD CODE - 'AND' OPERATOR ASSUMED '0288-13-7P(W)640288-14-'
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                 (640288-05-7P/RN)
               0 640288-06-8P
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                4-8P   640288-15-9P   640288-16-0P   640288-17-1P
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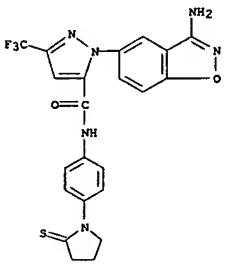
L13          12 640287-97-4 OR 640288-03-5 OR 640288-05-7 OR 640288-06-8 OR
                640288-07-9 OR 640288-11-5 OR 640288-12-6 OR 640288-13-7 OR
                640288-14-8 OR 640288-15-9 OR 640288-16-0 OR 640288-17-1

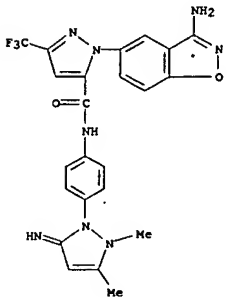
=> d sam 1-12
```

L13 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C22 H17 F3 N6 O2 S



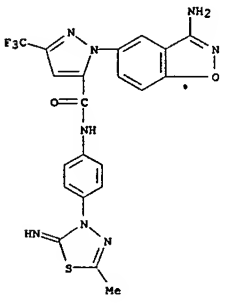
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2,5-dihydro-5-imino-2,3-dimethyl-1H-pyrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C23 H19 F3 N8 O2



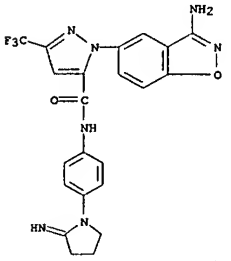
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C21 H15 F3 N8 O2 S



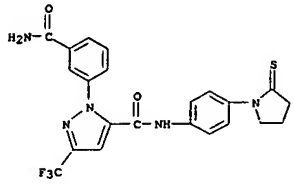
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C22 H18 F3 N7 O2



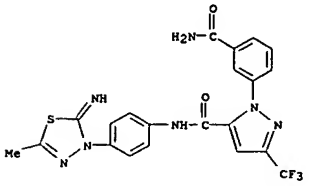
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C22 H18 F3 N5 O2 S



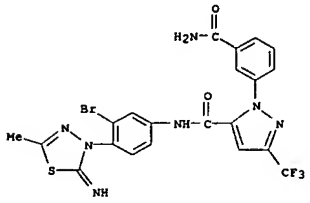
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C21 H16 F3 N7 O2 S



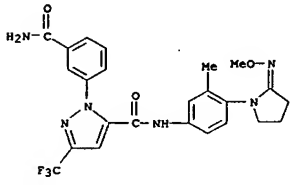
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-bromo-4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C21 H15 Br F3 N7 O2 S



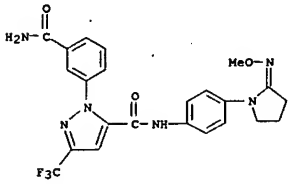
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]-3-methylphenyl]-3-(trifluoromethyl)- (9CI)
MF C24 H23 F3 N6 O3



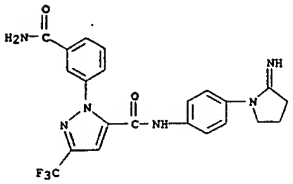
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI)
MF C23 H21 F3 N6 O3



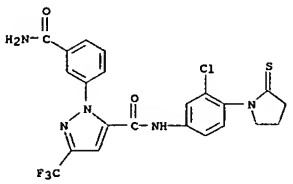
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C22 H19 F3 N6 O2



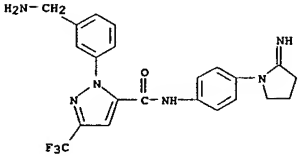
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-chloro-4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C22 H17 Cl F3 N5 O2 S



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L13 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI)
MF C22 H21 F3 N6 O . 2 Cl H



●2 HCl

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=> log h
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                   16.66     449.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    0.00     -35.88

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:13:37 ON 08 JAN 2007

Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:SSPTAJRK1626

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 10:03:28 ON 08 JAN 2007
FILE 'REGISTRY' ENTERED AT 10:03:28 ON 08 JAN 2007
COPYRIGHT (C) 2007 American Chemical Society (ACS)

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                   16.66     449.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    0.00     -35.88

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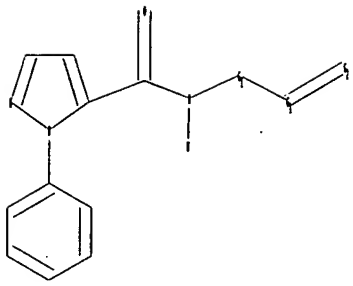
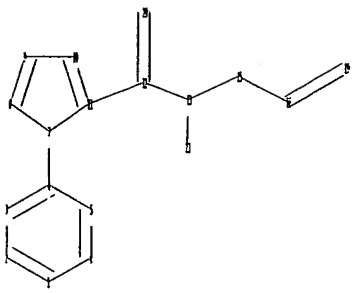




chain nodes :
12 13 15 16 19 20 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
4-7 11-12 12-13 12-20 13-15 13-21 15-16 16-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
4-7 7-8 7-11 8-9 9-10 10-11 12-13 12-20 13-15 15-16 16-19
exact bonds :
11-12 13-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

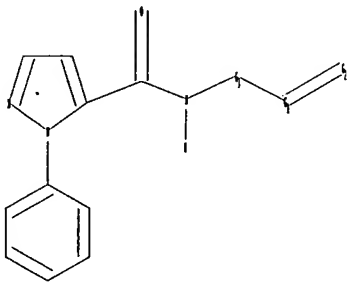
G1:Cb,Cy,Hy

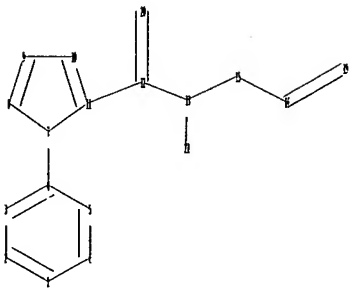
G2:S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS

L14 STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 8.str





chain nodes :
12 13 15 16 19 20 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
4-7 11-12 12-13 12-20 13-15 13-21 15-16 16-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
4-7 7-8 7-11 8-9 9-10 10-11 12-13 12-20 13-15 15-16 16-19

exact bonds :
11-12  13-21
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6

G1:Cb,Cy,Hy

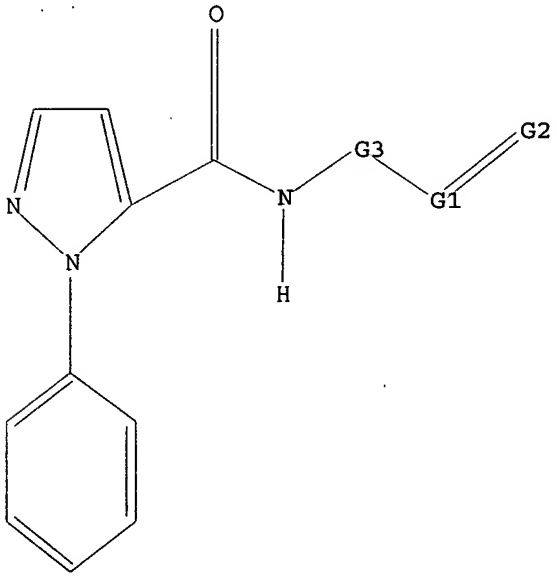
G2:S,N

G3:Cb,Cy,Hy,Ak

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:CLASS  13:CLASS  15:CLASS  16:CLASS  19:CLASS  20:CLASS  21:CLASS

L15  STRUCTURE UPLOADED

=> d
L15 HAS NO ANSWERS
L15  STR




G1 Cb,Cy,Hy
G2 S,N
G3 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> l15
SAMPLE SEARCH INITIATED 10:05:17 FILE 'REGISTRY'

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SAMPLE SCREEN SEARCH COMPLETED -      302 TO ITERATE

100.0% PROCESSED      302 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:          4998 TO     7082
PROJECTED ANSWERS:                1 TO       80

L16           1 SEA SSS SAM L15

=> l15 full
FULL SEARCH INITIATED 10:05:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     5859 TO ITERATE

100.0% PROCESSED     5859 ITERATIONS                               30 ANSWERS
SEARCH TIME: 00.00.01

L17          30 SEA SSS FUL L15

=> file medline caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   189.66     622.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -35.88

FILE 'MEDLINE' ENTERED AT 10:05:33 ON 08 JAN 2007

FILE 'CAPLUS' ENTERED AT 10:05:33 ON 08 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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=> l17
L18          5 L17

=> d ibib abs hitstr 1-5
```

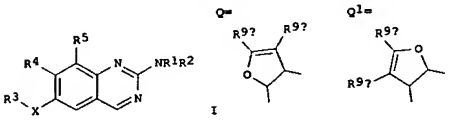
L18 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1176145 CAPLUS
DOCUMENT NUMBER: 145:489261
TITLE: Preparation of 2-aminoquinazoline derivatives as p38 mitogen-activated protein kinase inhibitors
INVENTOR(S): Kishikawa, Kuniyuki; Imase, Hidetomo; Kashima, Hajime; Mori, Kiyotoshi; Ikemura, Toshihide; Nakasato, Yoshisuke; Tomuro, Misato
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: PCT Int. Appl., 265pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2006118256 | A1 | 20061109 | WO 2006-JP309000 | 20060428 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: JP 2005-130704 A 20050428

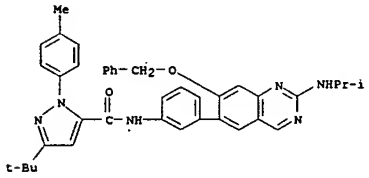
OTHER SOURCE(S): MARPAT 145:489261
GI



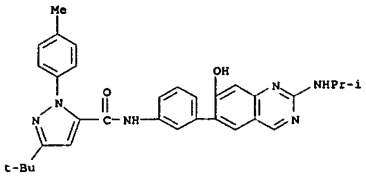

AB 2-Aminoquinazoline and 2-aminofuro[2,3-h]quinazoline derivs. represented by the general formula (I) or pharmacol. acceptable salts thereof [wherein R1, R2 = H, each (un)substituted lower alkyl, lower alkenyl, alkynyl, cycloalkyl, cycloalkenyl, lower alkanoyl, cycloalkylcarbonyl, aryl, heterocyclyl, CONH2; X = a bond, (un)substituted CH2; when X = a bond, R3 = (un)substituted aryl or aromatic heterocyclyl; when X = (un)substituted CH2, R3 = each (un)substituted lower alkoxy, aryl, arom. heterocyclyl, or CONH2; R4 = H, halo, HO, each (un)substituted lower alkyl, lower alkenyl, lower alkynyl, lower alkoxy, lower alkanoyloxy, aryl, aroyloxy, or heterocyclyl; R5 = H, halo, HO, each (un)substituted lower alkyl, lower alkenyl, lower alkoxy, aryl, heterocyclyl, or CONH2; or R4 and R5 together with the adjacent carbon atoms represent Q or Q1; R9a, R9b = H, halo, HO, each (un)substituted lower alkyl, lower alkenyl, lower alkoxy, lower alkoxycarbonyl, aryl, heterocyclyl, or CONH2] are prepd. These compds. are useful as p38 mitogen-activated protein (P38MAP) kinase inhibitors for the prevention and/or treatment of diseases related to the function of P38MAP kinase, e.g. inflammations, chronic articular rheumatism, osteoarthritis, arthritis, osteoporosis, autoimmune diseases, blood poisoning, cachexia, cerebral infarction, Alzheimer's disease, asthma, a chronic pneumonia, chronic obstructive pulmonary disease (COPD), thrombosis, glomerulonephritis, diabetes, host vs. graft rejection, inflammatory bowel disease, Crohn's disease, ulcerative colitis, multiple sclerosis, tumor proliferation and metastasis, multiple myeloma. Thus, 1.20 g 6-bromo-2-isopropylamino-7-methoxyquinazoline was dissolved in 20 mL dioxane and 20 mL H2O, treated with 0.900 g 2-chlorophenylboric acid, 1.03 g Na2CO3, and 197 mg [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium, and the resulting mixt. was heated under refluxing for 2 h to give, after workup and silica gel chromatog., 66% 6-(2-chlorophenyl)-2-isopropylamino-7-methoxyquinazoline (II). II at 1 μM inhibited ≥50% human P38MAP.

IT 914396-51-3P, 7-Benzyloxy-6-{3-[[[5-tert-butyl-2-(4-methylphenyl)-2H-pyrazol-3-yl]carbonyl]amino]phenyl]-2-(isopropylamino)quinazoline 914396-52-4P, 6-[3-[[[5-tert-Butyl-2-(4-methylphenyl)-2H-pyrazol-3-yl]carbonyl]amino]phenyl]-7-hydroxy-2-(isopropylamino)quinazoline
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-aminoquinazoline derivs. as p38 mitogen-activated protein kinase inhibitors)

RN 914396-51-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED




RN 914396-52-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



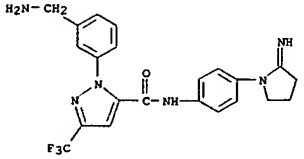

REFERENCE COUNT: 21 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
THERE ARE 21 CITED REFERENCES AVAILABLE FOR

L18 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1061760 CAPLUS
TITLE: Design and Evaluation of a Novel Class-Directed 2D Fingerprint to Search for Structurally Diverse Active Compounds
AUTHOR(S): Eckert, Hanna; Bajorath, Juergen
CORPORATE SOURCE: Department of Life Science Informatics, B-IT, Rheinische Friedrich-Wilhelms-Universitaet, Bonn, D-53113, Germany
SOURCE: Journal of Chemical Information and Modeling (2006), 46(6), 2515-2526
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Recent attempts to increase similarity search performance using mol. fingerprints have mostly focused on the evaluation of alternative similarity metrics or scoring schemes, rather than the development of new types of fingerprints. Here, the authors introduce a novel 2D fingerprint design (property descriptor value range-derived fingerprint or PDR-FP) that involves activity-oriented selection of property descriptors and the transformation of descriptor value ranges into a binary format such that each fingerprint bit position represents a specific value interval. The design is tailored toward multiple-template similarity searching and permits training on specific activity classes. In search calcns. on 15 compound classes of increasing structural diversity, the PDR fingerprint performed better than other state-of-the-art 2D fingerprints. Among the structurally diverse classes were six compound sets with peptide character, which represent a notoriously difficult chemotype for 2D similarity searching. In these cases, PDR-FP produced promising results, whereas other fingerprint methods mostly failed. PDR-FP is specifically designed for search calcns. on structurally diverse compds., and these calcns. are not influenced by mol. size effects, which represent a general problem for similarity searching using bit string representations.

IT 774536-86-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PRP (Properties); USES (Uses)
(design and evaluation of a class-directed 2D fingerprint to search for structurally diverse active compds.)

RN 774536-86-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L18 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:20490 CAPLUS
DOCUMENT NUMBER: 140:77148
TITLE: Preparation of N-[4-(thiooxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis
INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsaklakidis, Christos; Gleitz, Johannes; Barnes, Christopher
PATENT ASSIGNEE(S): Merck Patent Gmbh, Germany
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004002477 | A1 | 20040108 | WO 2003-EP5898 | 20030605 |
| WO 2004002477 | A8 | 20040415 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| DE 10229070 | A1 | 20040115 | DE 2002-10229070 | 20020628 |
| CA 2491271 | A1 | 20040108 | CA 2003-2491271 | 20030605 |
| AU 2003238475 | A1 | 20040119 | AU 2003-238475 | 20030605 |
| EP 1517685 | A1 | 20050330 | EP 2003-732540 | 20030605 |
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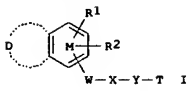
| JP 2005535630 | T | 20051124 | JP 2004-516575 | 20030605 |
| EP 1679073 | A1 | 20060712 | EP 2006-157 | 20030605 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, SK | | | | |
| US 2005203127 | A1 | 20050915 | US 2004-519356 | 20041228 |

PRIORITY APPLN. INFO.: DE 2002-10229070 A 20020628
EP 2003-732540 A3 20030605
WO 2003-EP5898 W 20030605

OTHER SOURCE(S): MARPAT 140:77148
GI

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



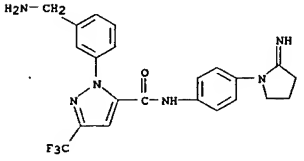
AB Title compds. [I; D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene; M = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(:S)N(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bi)cyclic aromatic (hetero)cyclyl; X = CONR3, CONR3C(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y = alkylene, cycloalkylene, heterodiyl, aryldiyl; T = (substituted) (bi)cyclic aromatic heterocyclyl], were prepared Thus, 333 mg

(3-[5-(4-[2-iminopyrrolidin-1-yl]phenylcarbamoyl)-3-trifluoromethylpyrazol-1-yl]benzyl)carbamic acid tert-Bu ester (preparation given) in EtOH was treated with HCl in ether to give 289 mg N-[4-(2-iminopyrrolidin-1-yl]phenyl]-1-(3-aminomethylphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the receptor Xa with IC50 = 9,6·10-9 M and to the receptor VIIa with IC50 = 2,3·10-8 M.

IT 640287-97-4P 640288-03-5P 640288-05-7P
640288-06-8P 640288-07-9P 640288-11-5P
640288-12-6P 640288-13-7P 640288-14-8P
640288-15-9P 640288-16-0P 640288-17-1P
640288-18-2P 640288-19-3P 640288-20-6P
640288-21-7P 640288-22-8P 640288-23-9P
640288-24-0P 640288-25-1P 640288-26-2P
640288-27-3P 640288-28-4P 640288-30-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

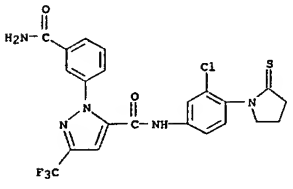
RN 640287-97-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

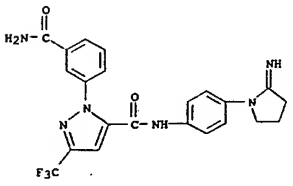


●2 HCl

RN 640288-03-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-chloro-4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

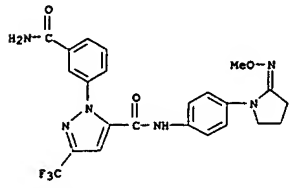


RN 640288-05-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

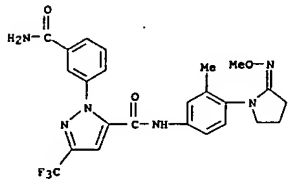


RN 640288-06-8 CAPLUS

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

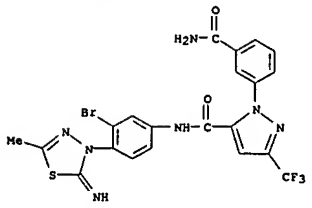


RN 640288-07-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]-3-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

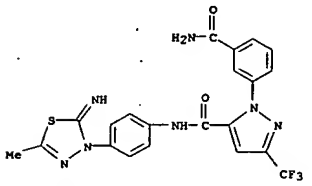


RN 640288-11-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-bromo-4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

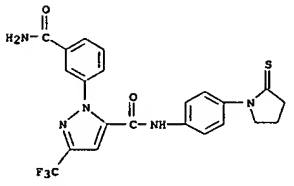


RN 640288-12-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

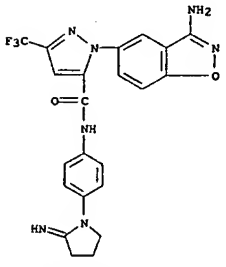


RN 640288-13-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

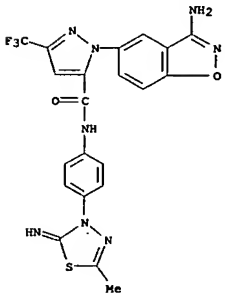


RN 640288-14-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

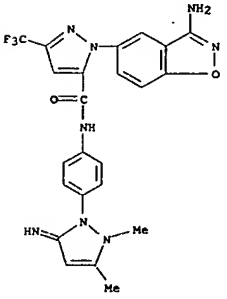


RN 640288-15-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

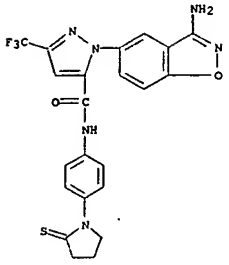


RN 640288-16-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2,5-dihydro-5-imino-2,3-dimethyl-1H-pyrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

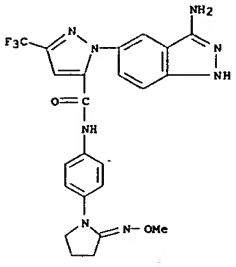


RN 640288-17-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

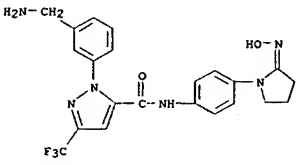


RN 640288-18-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1H-indazol-5-yl)-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

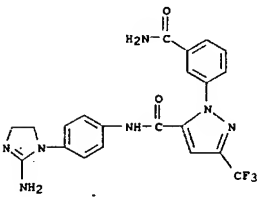


RN 640288-19-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1H-indazol-5-yl)-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

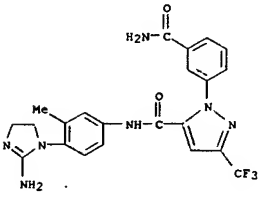
L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 640288-22-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-amino-4,5-dihydro-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

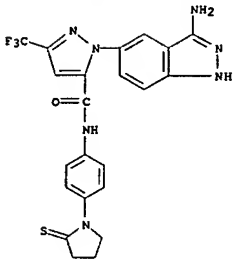


RN 640288-23-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-amino-4,5-dihydro-1H-imidazol-1-yl)-3-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

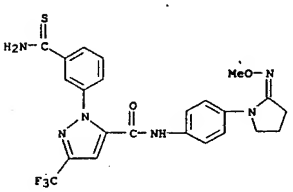


RN 640288-24-0 CAPLUS

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

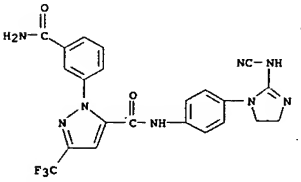


RN 640288-20-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminothioxomethyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

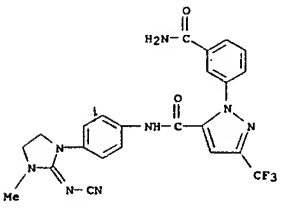


RN 640288-21-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[2-(hydroxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(cyanoamino)-4,5-dihydro-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

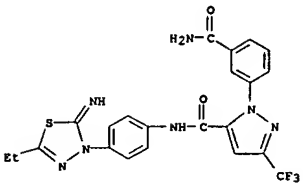


RN 640288-25-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(cyanoimino)-3-methyl-1-imidazolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

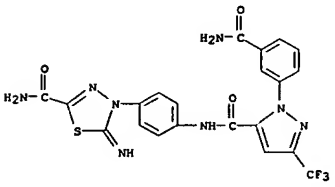


RN 640288-26-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(5-ethyl-2-imino-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

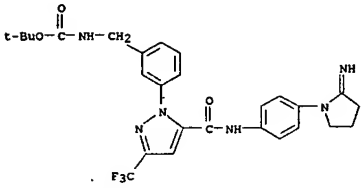


RN 640288-27-3 CAPLUS
CN 1,3,4-Thiadiazole-2-carboxamide, 4-[4-[[[1-[3-(aminocarbonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-4,5-dihydro-5-imino- (9CI) (CA INDEX NAME)



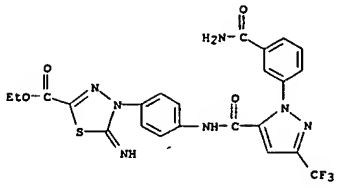
RN 640288-28-4 CAPLUS
CN 1,3,4-Thiadiazole-2-carboxylic acid, 4-[4-[[[1-[3-(aminocarbonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-4,5-dihydro-5-imino-, ethyl ester (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

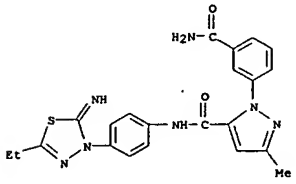


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 640288-30-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(5-ethyl-2-imino-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



IT 640288-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)
RN 640288-00-2 CAPLUS
CN Carbamic acid, [[3-[5-[[[4-(2-imino-1-pyrrolidinyl)phenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L18 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:39605 CAPLUS
DOCUMENT NUMBER: 136:102380
TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John M.; Han, Qi; Li, Renhua; Pinto, Donald J. P.; Pruitt, James R.; Quan, Mimi L.
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA
SOURCE: U.S., 117 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 6339099 | B1 | 20020115 | US 1998-99358 | 19980618 |
| US 2002025963 | A1 | 20020228 | US 2001-924381 | 20010808 |
| US 6906070 | B2 | 20050614 | | |
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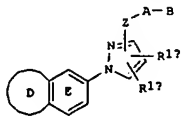
| US 6958356 | B2 | 20051025 | | |
| US 2004063772 | A1 | 20040401 | US 2003-602214 | 20030624 |
| US 6965036 | B2 | 20051115 | | |
| US 2006040973 | A1 | 20060223 | US 2005-197978 | 20050805 |

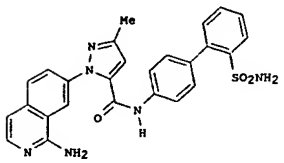
PRIORITY APPLN. INFO.: US 1997-50265P P 19970620
US 1998-99358 A3 19980618
US 2001-924381 B1 20010808
US 2002-98994 A1 20020313

OTHER SOURCE(S): MARPAT 136:102380
GI

L18 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



II

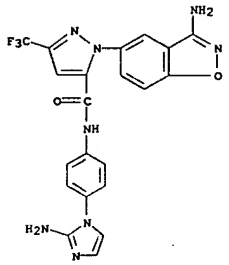


II

AB The title compds. [I; ring D = 5-membered aromatic system containing from 1-2 heteroatoms selected from N, O, S; ring D is substituted with 0-2 R groups; ring E contains 0-2 N atom and is substituted by 0-1 R groups; R = Cl, F, Br, I, OH, alkoxy, amino(alkyl), (alkyl)amino; Z = bond, alkylene, (CH2)rO(CH2)r, (CH2)rNR3(CH2)r, (CH2)rC(O)(CH2)r, (CH2)rC(O)O(CH2)r, (CH2)rOC(O)(CH2)r, (CH2)rC(O)NR3(CH2)r, etc. provided that Z does not form a N-N, N-O, N-S, NCH2N, NCH2O, or NCH2S bond with ring M or group A; R1a-1b = H, alk(en)yl, aminoalkyl, alkoxy, alternatively, R1a-1b, when attached to adjacent carbon atoms, together with the atoms to which they are attached form a 5-8 membered (un)saturated ring (un)substituted and which contains from 0-2 heteroatoms selected from the group consisting of N, O, and S; alternatively, when Z is C(O)NH and R1a is attached to a ring carbon adjacent to Z, then R1a is a C(O) which replaces the amide hydrogen of Z to form a cyclic imide; R3 = H, alkyl, phenyl; A = (un)substituted carbocyclic, 5-10 membered heterocyclic system containing 1-4 heteroatoms selected from N, O, S; B = H, Y, X-Y; X = sulfonylalkyl, alkylsulfonyl, sulfonamide, etc.; Y = alkylamino, provided that X-Y does not form a N-N, O-N or S-N bond, carbocyclic group, 5-10 membered heterocyclic r = 0-3], inhibitors of factor Xa which are useful in treating and preventing a thromboembolic disorder, were prepared and formulated. Thus, a multi-step synthesis of the title compound II, starting with 7-aminoisoquinoline, was described. A number of compds. I were found to exhibit a Ki of ≤ 15 μM against factor Xa.

IT 218298-55-6P 218299-98-0P

L18 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

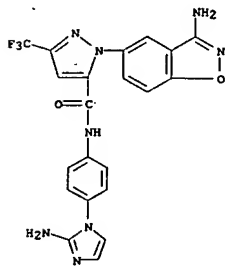
CRN 76-05-1
CMF C2 H F3 O2

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of novel guanidine mimics as factor Xa inhibitors)

RN 218298-55-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-amino-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 218299-98-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-amino-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 218298-55-6
CMF C21 H15 F3 N8 O2

L18 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:9833 CAPLUS
DOCUMENT NUMBER: 130:66494
TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John Matthew; Han, Qi; Li, Renhua; Pinto, Donald Joseph-Phillip; Pruitt, James Russell; Quan, Mimi Lifen
PATENT ASSIGNEE(S): The Du Pont Merck Pharmaceutical Company, USA
SOURCE: PCT Int. Appl., 268 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9857951 | A1 | 19981223 | WO 1998-US12680 | 19980618 |
| W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| ZA 9805247 | A | 19991217 | ZA 1998-5247 | 19980617 |
| CA 2291442 | A1 | 19981223 | CA 1998-2291442 | 19980618 |
| AU 9879768 | A | 19990104 | AU 1998-79768 | 19980618 |
| AU 756755 | B2 | 20030123 | | |
| EP 991638 | A1 | 20000412 | EP 1998-930361 | 19980618 |
| EP 991638 | B1 | 20050817 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO | | | | |
| BR 9810137 | A | 20000808 | BR 1998-10137 | 19980618 |
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| HU 200002686 | A2 | 20020128 | HU 2000-2686 | 19980618 |
| JP 2002505686 | T | 20020219 | JP 1999-504785 | 19980618 |
| NZ 502370 | A | 20021025 | NZ 1998-502370 | 19980618 |
| AT 302198 | T | 20050915 | AT 1998-930361 | 19980618 |
| ES 2244064 | T3 | 20051201 | ES 1998-930361 | 19980618 |
| RO 120543 | B1 | 20060330 | RO 1999-1317 | 19980618 |
| TW 544453 | B | 20030801 | TW 1998-87109910 | 19980819 |
| NO 9905965 | A | 19991203 | NO 1999-5965 | 19991203 |
| NO 318359 | B1 | 20050307 | | |
| MX 9911908 | A | 20000531 | MX 1999-11908 | 19991216 |
| LV 12496 | B | 20010120 | LV 1999-178 | 19991216 |
| LT 4705 | B | 20000925 | LT 1999-147 | 19991217 |
| PRIORITY APPLN. INFO.: | | | US 1997-878884 A | 19970619 |
| | | | WO 1998-US12680 W | 19980618 |

OTHER SOURCE(S): MARPAT 130:66494
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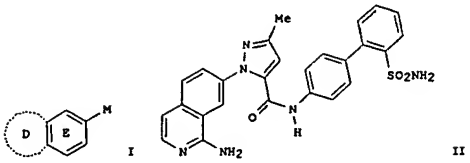
L18 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



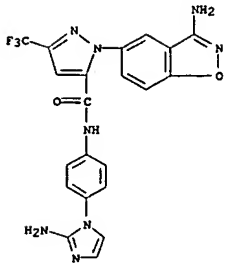
I II

AB The title compds. {I; rings D-E represent guanidine mimics; ring D = CH2N:CH, CH2CH2N:CH, a 5-6 membered aromatic system containing 0-2 heteroatoms selected form the group N, O, and S; ring D is substituted with 0-2 R (substituents), provided that when ring D is unsubstituted, it contains at least one heteroatom; ring E contains 0-2 N atom and is substituted by 0-1 R; R = halo, OH, C1-3 alkoxy, etc.; M = (un)substituted pyrazole, imidazole, tetrazole, etc.], inhibitors of factor Xa which are useful in treating and preventing a thromboembolic disorder, were prepared and formulated. Thus, a multi-step synthesis of the title compound II, starting with 7-aminoisoquinoline, was described. A number of compds. I were found to exhibit a Ki of ≤ 15 μM against factor Xa.

IT 218298-55-6P 218299-98-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel guanidine mimics as factor Xa inhibitors)

RN 218298-55-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-amino-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 218299-98-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-amino-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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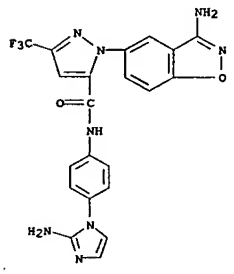
CRN 218298-55-6
CMF C21 H15 F3 N8 O2



L18 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2

CRN 76-05-1
CMF C2 H F3 O2

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FULL ESTIMATED COST                                    28.75     651.20

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -3.90     -39.78

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DICTIONARY FILE UPDATES:   7 JAN 2007  HIGHEST RN 916885-50-2

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http://www.cas.org/ONLINE/UG/regprops.html

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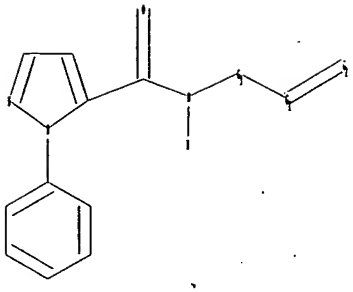

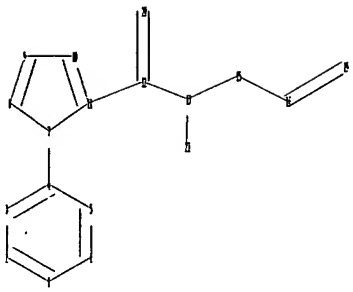

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ring nodes :
1 2 3 4 5 6 7 8 9 10 11
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ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
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exact bonds :
11-12 13-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:Cb,Cy,Hy

G2:S,N,O

G3:Cb,Cy,Hy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS

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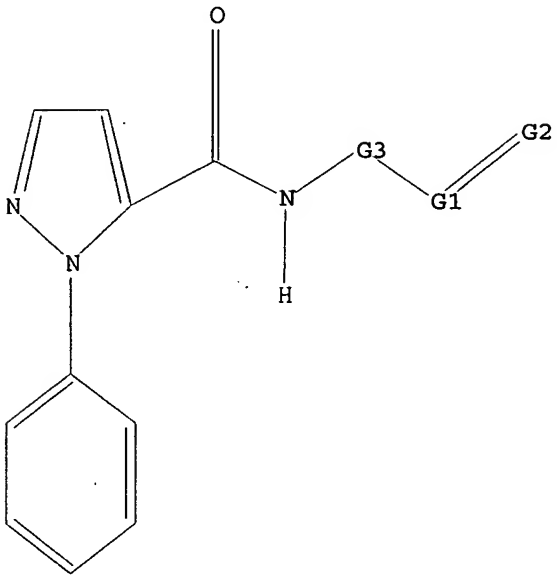
L19 STR




G1 Cb,Cy,Hy
G2 S,N,O
G3 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 319 TO ITERATE

100.0% PROCESSED 319 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5309 TO 7451
PROJECTED ANSWERS: 5 TO 234

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L20             5 SEA SSS SAM L19

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FULL SCREEN SEARCH COMPLETED -      6149 TO ITERATE

100.0% PROCESSED     6149 ITERATIONS                                 82 ANSWERS
SEARCH TIME: 00.00.01

L21           82 SEA SSS FUL L19

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FULL ESTIMATED COST                                   172.10     823.30

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                     0.00     -39.78

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=> l21
L22           11 L21

=> l22 not l18
L23            6 L22 NOT L18

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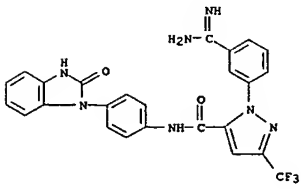
L23 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:791919 CAPLUS
DOCUMENT NUMBER: 141:342889
TITLE: SAR and factor IXa crystal structure of a dual inhibitor of factors IXa and Xa
AUTHOR(S): Smallheer, Joanne M.; Alexander, Richard S.; Wang, Jianmin; Wang, Shuaige; Nakajima, Suanne; Rossi, Karen A.; Smallwood, Angela; Barbera, Frank; Burdick, Debra; Luettgen, Joseph M.; Knabb, Robert M.; Wexler, Ruth R.; Jadhav, Prabhakar K.
CORPORATE SOURCE: Bristol-Myers Squibb Company, Princeton, NJ, 08543-5400, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(21), 5263-5267
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:342889
AB Modifications to the P4 moiety and pyrazole C3 substituent of factor Xa inhibitor SN-429 provided several new compds., which are 5-10 nM inhibitors of factor IXa. An x-ray crystal structure of one example complexed to factor IXa shows that these compds. adopt a similar binding mode to that previously observed with pyrazole inhibitors in the factor Xa active site both with regard to how the inhibitor binds and the position of Tyr99.
IT 848393-99-7P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(pyrazole compds. preparation, crystal structure, and dual inhibition of factors IXa and Xa)
RN 848393-99-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 774218-59-6
CMF C25 H18 F3 N7 O2

L23 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

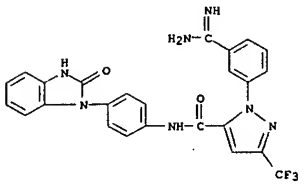


CM 2

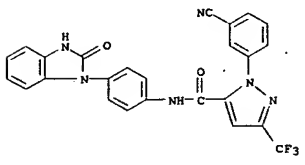
CRN 76-05-1
CMF C2 H F3 O2

IT 774218-59-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(pyrazole compds. preparation, crystal structure, and dual inhibition of factors IXa and Xa)
RN 774218-59-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

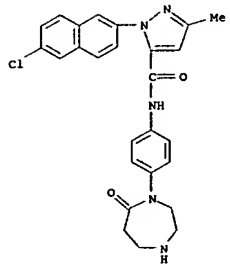


IT 848393-47-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(pyrazole compds. preparation, crystal structure, and dual inhibition of factors IXa and Xa)
RN 848393-47-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-cyanophenyl)-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

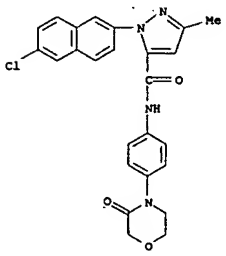


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:153586 CAPLUS
DOCUMENT NUMBER: 140:368084
TITLE: 1-(2-Naphthyl)-1H-pyrazole-5-carboxylamides as potent factor Xa inhibitors. Part 2: A survey of P4 motifs
AUTHOR(S): Jia, Zhaozhong J.; Wu, Yanhong; Huang, Wenrong; Zhang, Penglie; Clizbe, Lane A.; Goldman, Erick A.; Sinha, Uma; Arfsten, Ann E.; Edwards, Susan T.; Alphonso, Merlyn; Hutchaleelaha, Athiwat; Scarborough, Robert M.; Zhu, Bing-Yan
CORPORATE SOURCE: Millennium Pharmaceuticals, Inc., South San Francisco, CA, 94080, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(5), 1221-1227
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A variety of P4 motifs have been examined to increase the binding affinity and in vitro anticoagulant potency of our biphenyl 1-(2-naphthyl)-1H-pyrazole-5-carboxylamide-based fXa inhibitors. Highly potent 2-naphthyl-P1 fXa inhibitors (Ki≤2 nM) with improved in vitro anticoagulant activity (2+TGS1 μM) and respectable pharmacokinetic properties have been discovered.
IT 684233-39-4 684233-40-7 684233-41-8
684233-42-9 684233-66-7 684233-70-3
684233-71-4 684233-72-5 684233-73-6
684233-74-7 684233-75-8
RL: PAC (Pharmacological activity); BIOL (Biological study)
(1-(2-Naphthyl)-1H-pyrazole-5-carboxylamides as potent factor Xa inhibitors)
RN 684233-39-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(6-chloro-2-naphthalenyl)-N-[4-(hexahydro-7-oxo-1H-1,4-diazepin-1-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 684233-40-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(6-chloro-2-naphthalenyl)-3-methyl-N-[4-(3-oxo-4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 684233-41-8 CAPLUS
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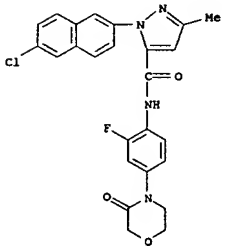

RN 684233-42-9 CAPLUS
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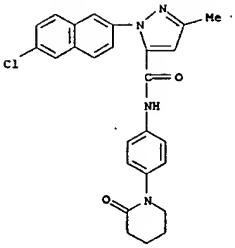
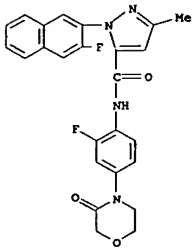
L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

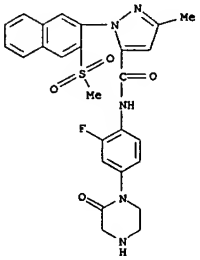


RN 684233-66-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-fluoro-2-naphthalenyl)-N-[2-fluoro-4-(3-oxo-4-morpholinyl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)

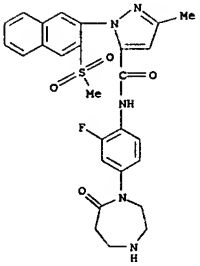


RN 684233-70-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(2-oxo-1-piperazinyl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

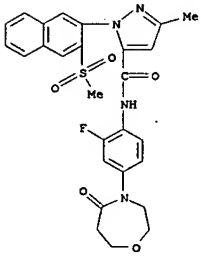


RN 684233-71-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[2-fluoro-4-(hexahydro-7-oxo-1H-1,4-diazepin-1-yl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

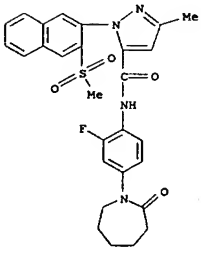


RN 684233-72-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(tetrahydro-5-oxo-1,4-oxazepin-4(5H)-yl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

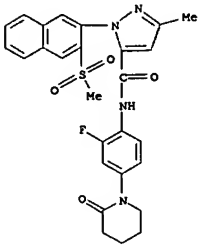


RN 684233-73-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(hexahydro-2-oxo-1H-azepin-1-yl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

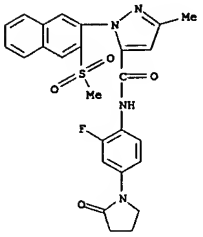


RN 684233-74-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(2-oxo-1-piperidinyl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

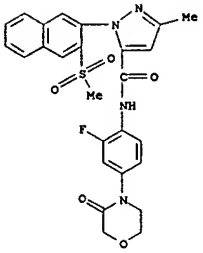


RN 684233-75-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(2-oxo-1-pyrrolidinyl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)



IT 684233-69-0
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); BIOL (Biological study)
(1-(2-Naphthyl)-1H-pyrazole-5-carboxylamides as potent factor Xa inhibitors)
RN 684233-69-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(3-oxo-4-morpholinyl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

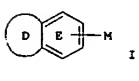
L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:725629 CAPLUS
DOCUMENT NUMBER: 133:296430
TITLE: Preparation of aryl sulfonyls as factor Xa inhibitors
INVENTOR(S): Wexler, Ruth R.; Jacobson, Irina C.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000059902 | A2 | 20001012 | WO 2000-US8364 | 20000330 |
| WO 2000059902 | A3 | 20010426 | | |
| W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| CA 2368630 | A1 | 20001012 | CA 2000-2368630 | 20000330 |
| EP 1175419 | A2 | 20020130 | EP 2000-923096 | 20000330 |
| EP 1175419 | B1 | 20030528 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| AT 241621 | T | 20030615 | AT 2000-923096 | 20000330 |
| ES 2197092 | T3 | 20040101 | ES 2000-923096 | 20000330 |
| US 6399644 | B1 | 20020604 | US 2000-540467 | 20000331 |
| US 2003050315 | A1 | 20030313 | US 2002-74301 | 20020212 |
| US 6689770 | B2 | 20040210 | | |

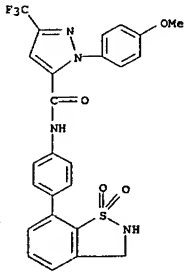
PRIORITY APPLN. INFO.: US 1999-127634P P 19990402
WO 2000-US8364 W 20000330
US 2000-540467 A3 20000331

OTHER SOURCE(S): MARPAT 133:296430
GI



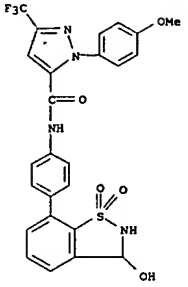
AB Aryl sulfonyls I [ring D is absent or is CH2N:CH, CH:NCH2, aromatic system
containing heteroatoms, etc.; E = Ph, pyridyl, pyrazinyl, etc.; M = heterocyclyl], effective factor Xa inhibitors (no data), were prepared E.g., N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide was prepared
IT 300710-13-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Reactant or reagent); USES (Uses)
(prepn. of aryl sulfonyls as factor Xa inhibitors)
RN 300710-13-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)-(9CI)
(CA INDEX NAME)

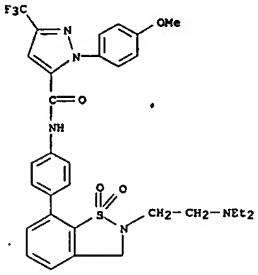


IT 300710-14-9P 300710-15-0P 300710-16-1P
300710-17-2P 300710-18-3P 300710-19-4P
300710-20-7P 300710-21-8P 300710-22-9P
300710-23-0P 300710-24-1P 300710-25-2P
300710-26-3P 300710-27-4P 300710-28-5P
300710-29-6P 300710-30-9P 300710-31-0P
300710-32-1P 300710-33-2P 300710-34-3P
300710-35-4P 300710-36-5P 300710-37-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl sulfonyls as factor Xa inhibitors)
RN 300710-14-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-(2,3-dihydro-3-hydroxy-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)-(9CI)
(CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

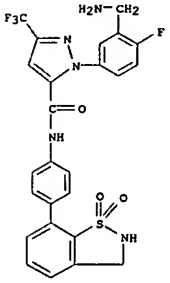


RN 300710-15-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-[2-[2-(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

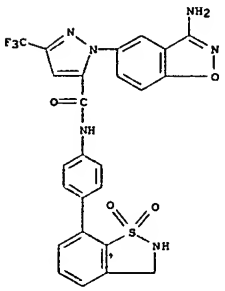


RN 300710-16-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

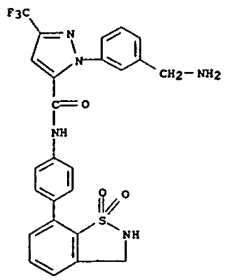


RN 300710-19-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

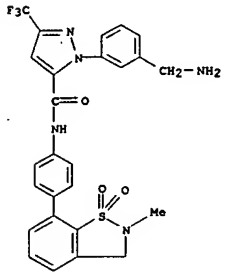


RN 300710-20-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-[2-(cyanomethyl)-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
INDEX NAME)

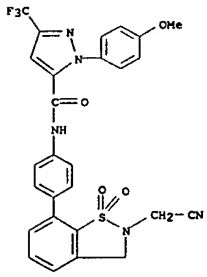


RN 300710-17-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

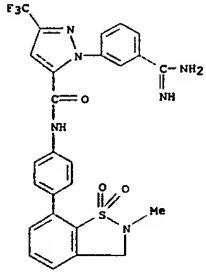


RN 300710-18-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

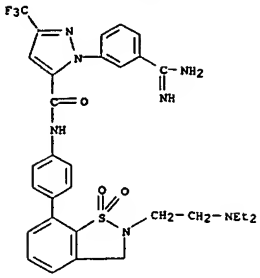


RN 300710-21-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

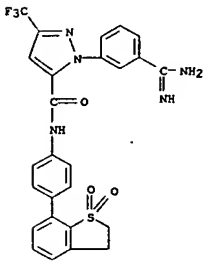


RN 300710-22-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-[2-[2-(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

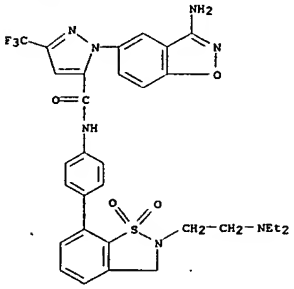


RN 300710-23-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxidobenzo[b]thien-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

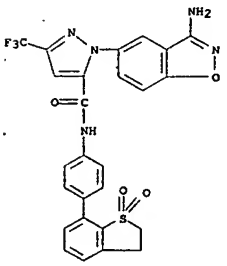


RN 300710-24-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxidobenzo[b]thien-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

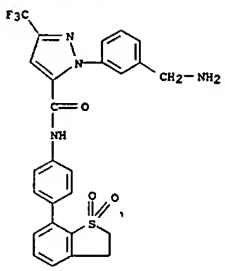


RN 300710-27-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2,3-dihydro-1,1-dioxidobenzo[b]thien-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

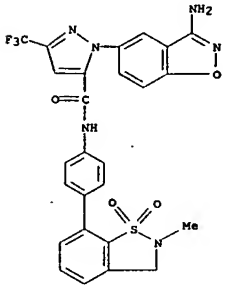


RN 300710-28-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[2-[2-(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

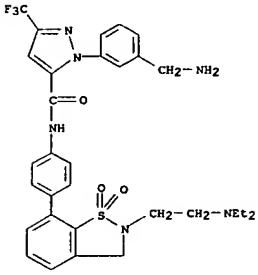


RN 300710-25-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

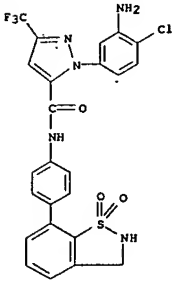


RN 300710-26-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-[2-[2-(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

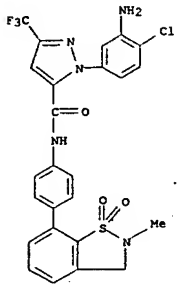


RN 300710-29-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-4-chlorophenyl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

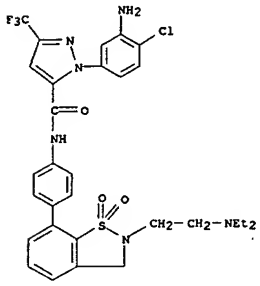


RN 300710-30-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-4-chlorophenyl)-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

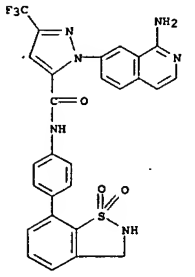


RN 300710-31-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-4-chlorophenyl)-N-[4-[2-[2-(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

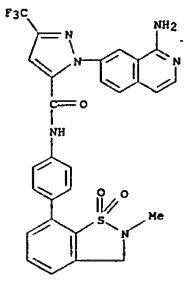


RN 300710-32-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-4-chlorophenyl)-N-[4-(2,3-dihydro-1,1-dioxidobenzo[b]thien-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

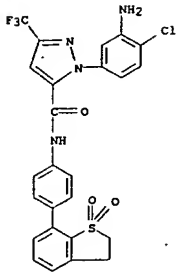


RN 300710-35-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

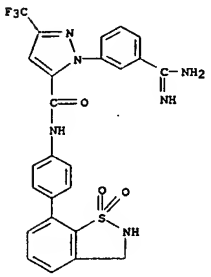


RN 300710-36-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[4-[2-[2-(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

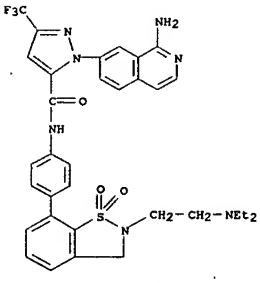


RN 300710-33-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

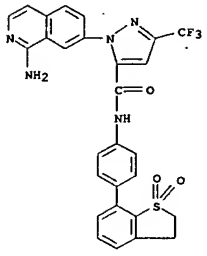


RN 300710-34-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

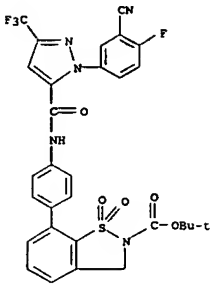


RN 300710-37-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[4-(2,3-dihydro-1,1-dioxidobenzo[b]thien-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

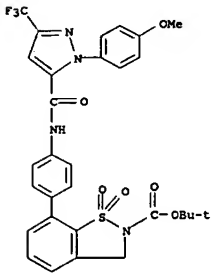


IT 300710-47-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aryl sulfonyls as factor Xa inhibitors)
RN 300710-47-8 CAPLUS
CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-(3-cyano-4-fluorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

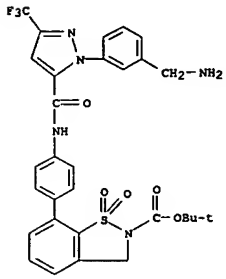


IT 300710-44-5P 300710-45-6P 300710-46-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl sulfonyls as factor Xa inhibitors)
RN 300710-44-5 CAPLUS
CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-(4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

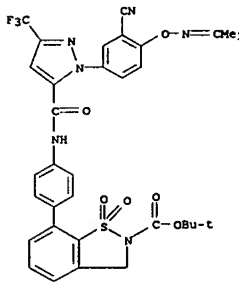


RN 300710-45-6 CAPLUS

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)



RN 300710-46-7 CAPLUS
CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-[3-cyano-4-[[(1-methylethylidene)amino]oxy]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)



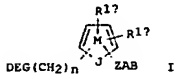
L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:83115 CAPLUS
DOCUMENT NUMBER: 132:137392
TITLE: Preparation of azoles as Factor Xa inhibitors.
INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell; Cacciola, Joseph; Fevig, John Matthew; Han, Qi; Orwat, Michael James; Quan, Mimi Lifen; Rossi, Karen Anita
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Co., USA
SOURCE: U.S., 152 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

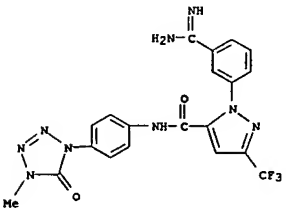
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 6020357 | A | 20000201 | US 1997-995834 | 19971222 |
| US 6548512 | B1 | 20030415 | US 2000-492708 | 20000127 |
| PRIORITY APPLN. INFO.: | | | US 1996-33437P | P 19961223 |
| | | | US 1997-50304P | P 19970620 |
| | | | US 1997-995834 | A3 19971222 |

OTHER SOURCE(S): MARPAT 132:137392
GI



AB Title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(:NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = C1-4 alkylene, (CH2)rO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2; with provisos], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded 1-(3-amidinophenyl)-2-[(2'-aminosulfonyl-1,1'-biphen-4-yl)aminocarbonyl]imidazole. Several I showed Ki ≤10 μM against

L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Factor Xa and thrombin.
IT 209956-77-4P 209956-78-5P 209958-09-8P
209958-10-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azoles as Factor Xa inhibitors)
RN 209956-77-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-(9CI)
(CA INDEX NAME)



RN 209956-78-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

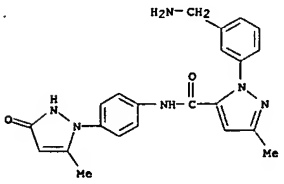
CM 1

CRN 209956-77-4
CMF C20 H16 F3 N9 O2

L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)

CM 1

CRN 209958-09-8
CMF C22 H22 N6 O2

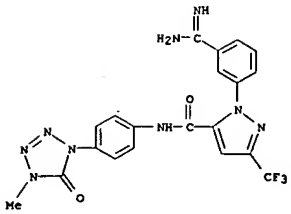


CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 209959-74-0P 209960-49-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azoles as Factor Xa inhibitors)
RN 209959-74-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-cyanophenyl)-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

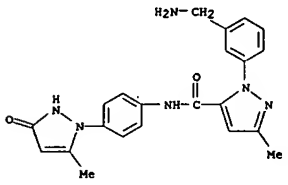
L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

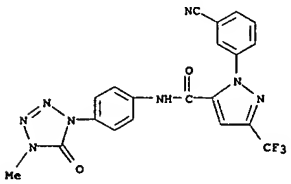
CRN 76-05-1
CMF C2 H F3 O2

RN 209958-09-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)

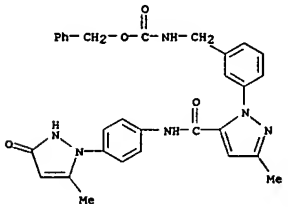


RN 209958-10-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl-, mono(trifluoroacetate)

L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209960-49-6 CAPLUS
CN Carbamic acid, [[3-[5-[[[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]amino]carbonyl]-3-methyl-1H-pyrazol-1-yl]phenyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

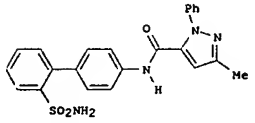


REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:9820 CAPLUS
DOCUMENT NUMBER: 130:81510
TITLE: Preparation of phenylpyrazolecarboxamides as coagulation factor Xa inhibitors
INVENTOR(S): Galemmo, Robert Anthony, Jr.; Dominguez, Celia; Fevig, John Matthew; Han, Qi; Lam, Patrick Yuk-sun; Pinto, Donald Joseph Philip; Pruitt, James Russell; Quan, Mimi Lifen
PATENT ASSIGNEE(S): The Du Pont Merck Pharmaceutical Company, USA
SOURCE: PCT Int. Appl., 259 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

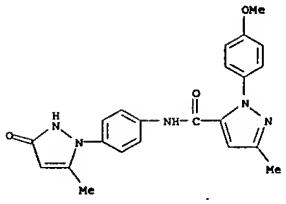
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9857937 | A2 | 19981223 | WO 1998-US12681 | 19980618 |
| WO 9857937 | A3 | 19990318 | | |
| W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| ZA 9805251 | A | 19991217 | ZA 1998-5251 | 19980617 |
| CA 2290982 | A1 | 19981223 | CA 1998-2290982 | 19980618 |
| AU 9881503 | A | 19990104 | AU 1998-81503 | 19980618 |
| US 5998424 | A | 19991207 | US 1998-99752 | 19980618 |
| EP 991625 | A2 | 20000412 | EP 1998-931355 | 19980618 |
| EP 991625 | B1 | 20050601 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO | | | | |
| BR 9810151 | A | 20000808 | BR 1998-10151 | 19980618 |
| EE 9900584 | A | 20000815 | EE 1999-584 | 19980618 |
| SI 20208 | A | 20001031 | SI 1998-20043 | 19980618 |
| HU 200003906 | A2 | 20010528 | HU 2000-3906 | 19980618 |
| JP 2002507968 | T | 20020312 | JP 1999-504786 | 19980618 |
| AT 296805 | T | 20050615 | AT 1998-931355 | 19980618 |
| ES 2239806 | T3 | 20051001 | ES 1998-931355 | 19980618 |
| PT 991625 | T | 20051031 | PT 1998-931355 | 19980618 |
| US 6403620 | B1 | 20020611 | US 1999-393782 | 19990910 |
| LV 12516 | B | 20010320 | LV 1999-177 | 19991216 |
| NO 9906316 | A | 19991217 | NO 1999-6316 | 19991217 |
| LT 4702 | B | 20000925 | LT 1999-146 | 19991217 |
| WO 2001080762 | A2 | 20011101 | WO 2001-US13280 | 20010424 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2002106604 | A1 | 20020808 | US 2001-40269 | 20011029 |
| US 6705863 | B2 | 20040316 | | |
| US 2003092740 | A1 | 20030515 | US 2002-150698 | 20020516 |
| US 6602895 | B2 | 20030805 | | |
| US 7059850 | B1 | 20060613 | US 2003-632482 | 20030801 |
| US 2004048223 | A1 | 20040311 | US 2003-660857 | 20030912 |
| US 7125248 | B2 | 20061024 | | |
| US 2004110110 | A1 | 20040610 | US 2003-718779 | 20031120 |
| US 7134874 | B2 | 20061114 | | |
| US 2004209218 | A1 | 20041021 | US 2004-799432 | 20040312 |
| US 7121825 | B2 | 20061017 | | |
| JP 2005118592 | A | 20050512 | JP 2004-341318 | 20041125 |
| PRIORITY APPLN. INFO.: | | | US 1997-50219P | P 19970619 |
| | | | US 1997-878885 | A 19970619 |
| | | | US 1998-76691P | P 19980227 |
| | | | US 1997-50342P | P 19970620 |
| | | | US 1997-947080 | A2 19971008 |
| | | | US 1998-99752 | A3 19980618 |
| | | | WO 1998-US12681 | W 19980618 |
| | | | WO 1998-US12861 | A1 19980619 |
| | | | US 1998-169034 | A2 19981008 |
| | | | US 1998-169276 | B1 19981008 |
| | | | US 1998-110189P | P 19981130 |
| | | | US 1998-110881P | P 19981204 |
| | | | US 1999-250962 | A2 19990216 |
| | | | US 1999-393782 | A3 19990910 |
| | | | JP 2000-584831 | A3 19991123 |
| | | | US 1999-454278 | A2 19991203 |
| | | | US 1999-466353 | A2 19991217 |
| | | | US 2000-199649P | P 20000425 |
| | | | US 2000-199650P | P 20000425 |
| | | | US 2000-616222 | A2 20000714 |
| | | | US 2000-686190 | B1 20001010 |
| | | | US 2001-757385 | A1 20010108 |
| | | | WO 2001-US13280 | A2 20010424 |
| | | | US 2001-40269 | A1 20011029 |
| | | | US 2002-99187 | A1 20020313 |
| | | | US 2002-139153 | A2 20020502 |
| | | | US 2002-262516 | A2 20020930 |

OTHER SOURCE(S): MARPAT 130:81510
GI




II

AB EZlM [I; E = halo, OH, alkyl, alkoxy, etc.; M = Z2ZAB; A = (un)substituted carbocyclylene, -heterocyclylene; B = H, Y, XY; X = alkylene, CO, O, (un)substituted NH, etc.; Y = amino(alkyl), substituted carbocyclyl, -heterocyclyl, etc.; Z = bond, (heteroatom- or functional group-interrupted) alkylene, etc.; Z1 = (un)substituted Ph, Z2 = N-containing heteroarylene, etc.] were prepared Thus, MeCOCH2C(:NOMe)CO2Et was cyclocondensed with PhNHNH2 and the product amidated by 4-(H2N)C6H4C6H4(SO2NHCMe3)-2 to give, after deprotection, title compound II.
Data for biol. activity of I were given.
IT 218630-82-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylpyrazolecarboxamides as coagulation factor Xa inhibitors)
RN 218630-82-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-1-(4-methoxyphenyl)-3-methyl- (9CI) (CA INDEX NAME)



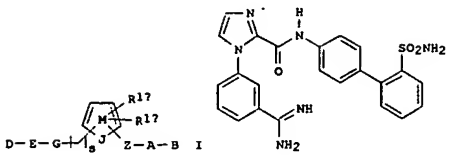
L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:479506 CAPLUS
DOCUMENT NUMBER: 129:109090
TITLE: Preparation of nitrogen-containing heteroaromatics as factor Xa inhibitors
INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell; Cacciola, Joseph; Fevig, John Matthew; Han, Qi; Orwat, Michael James; Quan, Mimi Lifen; Rossi, Karen Anita
PATENT ASSIGNEE(S): The Dupont Merck Pharmaceutical Co., USA
SOURCE: PCT Int. Appl., 438 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9828269 | A1 | 19980702 | WO 1997-US22895 | 19971215 |
| W: AM, AU, AZ, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KG, KR, KZ, LT, LV, MD, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, UA, VN | | | | |
| RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| CA 2275796 | A1 | 19980702 | CA 1997-2275796 | 19971215 |
| AU 9856020 | A | 19980717 | AU 1998-56020 | 19971215 |
| AU 730224 | B2 | 20010301 | | |
| EP 946508 | A1 | 19991006 | EP 1997-952409 | 19971215 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI | | | | |
| EE 9900316 | A | 20000215 | EE 1999-316 | 19971215 |
| SI 20017 | A | 20000229 | SI 1997-20082 | 19971215 |
| CN 1246847 | A | 20000308 | CN 1997-181852 | 19971215 |
| BR 9714073 | A | 20000509 | BR 1997-14073 | 19971215 |
| HU 200000735 | A2 | 20010428 | HU 2000-735 | 19971215 |
| JP 2001509145 | T | 20010710 | JP 1998-528845 | 19971215 |
| ZA 9711586 | A | 19990701 | ZA 1997-11586 | 19971223 |
| TW 492971 | B | 20020701 | TW 1997-86119637 | 19980203 |
| NO 9902633 | A | 19990820 | NO 1999-2633 | 19990601 |
| NO 313190 | B1 | 20020826 | | |
| MX 9905878 | A | 20000131 | MX 1999-5878 | 19990622 |
| LT 4673 | B | 20000725 | LT 1999-76 | 19990622 |
| LV 12430 | B | 20000720 | LV 1999-99 | 19990730 |

PRIORITY APPLN. INFO.: US 1996-769859 A 19961223
US 1997-879944 A 19970620
WO 1997-US22895 W 19971215

OTHER SOURCE(S): MARPAT 129:109090
GI

L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

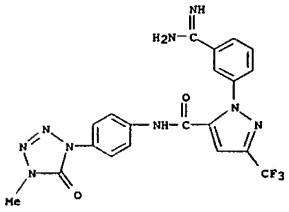


AB The title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(:NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = C1-4 alkylene, (CH2)rO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2C12 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded the title compound II. A number of compds. I were found to exhibit a Ki of ≤ 10 μM against factor Xa. Some compds. I were evaluated and found to exhibit Ki of < 10 μM against thrombin.

IT 209956-77-4P 209956-78-5P 209958-09-8P
209958-10-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)

RN 209956-77-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

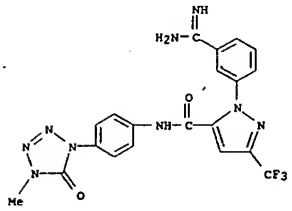
L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209956-78-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-77-4
CMF C20 H16 F3 N9 O2

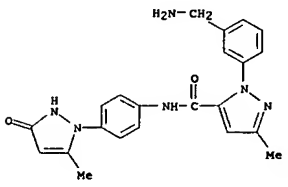


CM 2

CRN 76-05-1
CMF C2 H F3 O2

L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

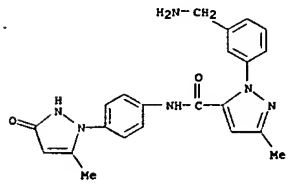
RN 209958-09-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209958-10-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-09-8
CMF C22 H22 N6 O2

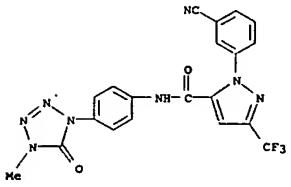


CM 2

CRN 76-05-1
CMF C2 H F3 O2

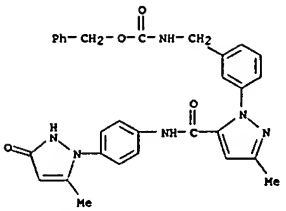
L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 209959-74-0P 209960-49-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)
RN 209959-74-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-cyanophenyl)-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209960-49-6 CAPLUS
CN Carbamic acid, [[3-[5-[[[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]amino]carbonyl]-3-methyl-1H-pyrazol-1-yl]phenyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FULL ESTIMATED COST                                    35.53     858.83

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -4.68     -44.46

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:11:39 ON 08 JAN 2007
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